ABSTRACTS

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MONDAY, MARCH 10

PLENARIES

MOOSE: A Retrospective

Derek Gaston, U.S. Department of Energy

This talk examines how MOOSE (Multiphysics Object-Oriented Simulation Environment) emerged from Idaho National Laboratory to address the need for accessible, powerful computational tools. MOOSE's innovative design freed scientists from coding complexities, allowing them to focus on physics rather than parallel computing or numerical methods. We'll explore how its object-oriented architecture, flexible coupling capabilities, and amazing team transformed scientific simulation, evolving from a specialized tool into a vibrant ecosystem serving diverse disciplines from nuclear engineering to materials science.

MOOSE: What's next?

Cody Permann, Idaho National Laboratory

For almost seventeen years, the MOOSE framework has facilitated swift and effective multiphysics modeling and simulation. As the next generation of reactors are demonstrated and deployed, many in the computational science computing are wondering what's next. We anticipate that the framework will evolve into new application areas, integrate emerging technologies, and explore entirely new uses. This keynote will showcase both current and prospective technologies and application domains that we are investigating and aim to explore.

The U.S. Nuclear Regulatory Commission Approach to Modeling and Simulation of Advanced Non-LWRs; Preparing for Today's Nuclear Renaissance

Steve Bajorek, U.S. Nuclear Regulatory Commission

There is considerable interest in the U.S. and internationally in advanced non-light water reactors to provide abundant carbon-free energy, and for their potential to replace existing, yet aging, conventional nuclear units. Energy demands for data centers add to the need. A significant number of conventional power plants are expected to retire over the two decades. Replacement of this capacity is necessary but offers an opportunity to new nuclear capacity. Numerous designers are responding to the opportunity. Advanced non-LWR designs utilizing a variety of coolants; gas, liquid metal, molten salt, are under development. Preliminary estimates are that these new designs can improve safety, improve economics, and provide capabilities not possible with conventional designs. The U.S. NRC is responding to this changing environment by updating its licensing process and by preparing for its review of non-LWRs. The NRC has developed a vision and strategy to assure that the NRC is ready to review potential applications for non-light water reactor (non-LWR) technologies effectively and efficiently [1]. The strategy consists of six strategic areas:

1. staff development and knowledge management
2. analytical tools

3. regulatory framework
4. consensus codes and standards
5. resolution of policy issues
6. communications

The purpose of this presentation is to discuss and focus on strategic area #2; analytical tools. As pointed out in the vison and strategy document, “The staff must have adequate computer models and other analytical resources to conduct its review of non-LWR designs in an independent manner”. But lacking existing tools and methods for non-LWR analysis the NRC decided to adopt a several analysis codes developed as part of the MOOSE Framework. The combination of the MOOSE developed codes and NRC developed codes resulted in an analysis suite of tools referred to as “BlueCRAB” for the (Federal) Comprehensive Reactor Analysis Bundle. This presentation provides a brief history of BlueCRAB, summarizes the current status and discusses future needs and development.

Fusion Panel

Casey Icenhour (Idaho National Laboratory, INL), Pierre-Clement Simon (INL), Andy Davis (United Kingdom Atomic Energy Authority), Carlo Fiorina (Texas A&M University)

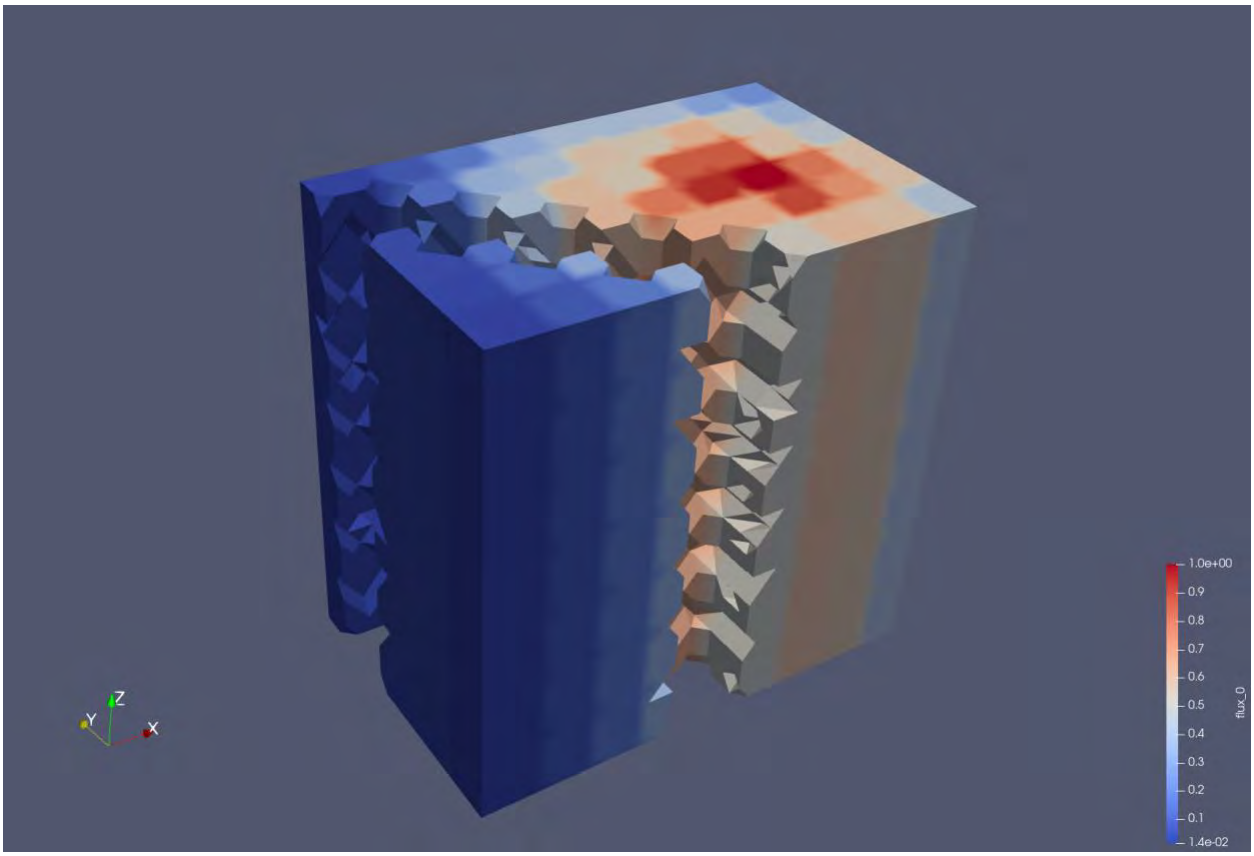
In this panel, computational fusion experts will discuss how MOOSE and MOOSE based tools have been and can be used to accelerate the deployment of fusion technologies and fusion energy.

NUCLEAR 1

MOOSE equivalence calculation for a multigroup model of neutron albedo

Gabriel Burgio (Research Neutron Source Heinz Maier-Leibnitz, FRM II), Christian Reiter (FRM II)

We developed an extension to the hybrid SPH-DF equivalence procedure for the multigroup diffusion equation that was already investigated in MOOSE by INL scientists. Our approach includes explicit modeling of the reflector through the use of array albedo boundary conditions (that generalize the standard reflective and vacuum cases through the use of an albedo matrix), and the computation of corrective factors for the returning albedo currents. Explicit reflector treatment allows for the exclusion of the reflector and all other material zones surrounding the fuel from the computational domain, reducing computational cost and potentially greatly simplifying meshing. We carried out a thorough mathematical analysis of the model with the newly derived boundary conditions to establish well-posedness, and obtained new results regarding the conditions necessary for the normalization factors to converge to the same value across groups, which gives the reproduction of reference fluxes and boundary currents in the homogenized model. We showed these conditions to be automatically satisfied in the classical cases of vacuum and reflective boundaries. The procedure was benchmarked in MOOSE on a Serpent 2 model of the MNR reactor, reproducing reference criticality eigenvalues to within a few pcms.

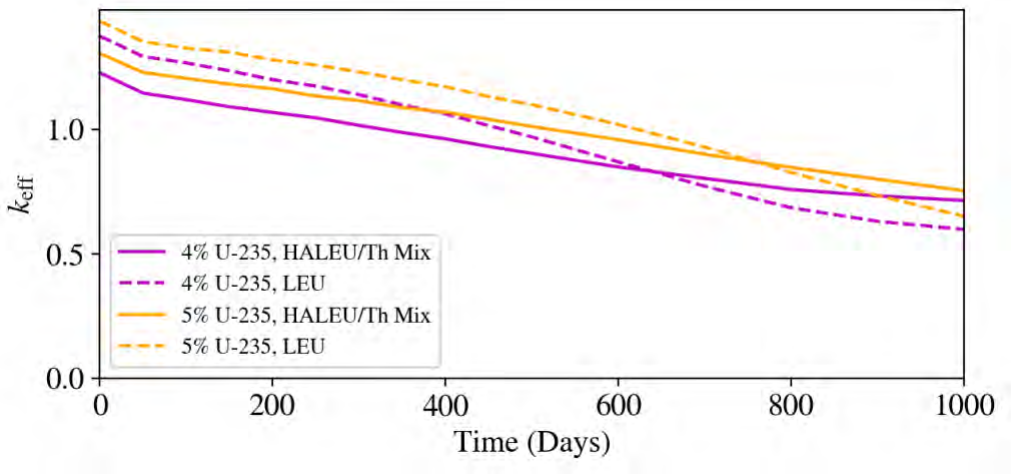


Multiphysics and Multiscale Simulation using Cardinal

April Novak (University of Illinois, Urbana-Champaign, UIUC), A. Hegazy (UIUC), M. Eltawila (UIUC), M. Elkamash (UIUC), T. Labossiere-Hickman (INL/UIUC), M. Mendes (UIUC), K. Sawatzky (UIUC), J. Specht (UIUC), N. Glaser (UIUC), S. Siewert (UIUC), N. Purohit (UIUC), O. Evans (UIUC)

Recent growth in computing now permits large-scale multiphysics and multiscale modeling using Monte Carlo neutron-photon transport and computational fluid dynamics (CFD), considered state-of-the-art for radiation transport and thermal-fluids. The enormous diversity in the advanced reactor landscape requires a flexible and general-purpose computational framework. Cardinal is an open-source, high-fidelity MOOSE application which integrates OpenMC Monte Carlo radiation transport and NekRS spectral element CFD with the MOOSE ecosystem. High-fidelity analysis plays an important role in benchmarking coarse-mesh codes, identifying physics/methods knowledge gaps, and generating constitutive models. This talk will describe recent research at the University of Illinois in the application and development of multiphysics/multiscale simulation using Cardinal. First, we will describe recent developments to couple Monte Carlo methods with moving-mesh thermomechanics for evaluation of reactivity and streaming effects from geometry motion. OpenMC's surface mesh-based geometry is integrated with the MOOSE thermomechanics module, with physics-driven geometry changes updated on-the-fly for radiation transport. Next, we describe mixed coupling of body-fitted and immersed boundary methods for reducing upfront meshing time for thermal-fluid simulation. This work will be shown coupling NekRS with immersed boundary techniques to body-fitted MOOSE meshes for pebble bed reactor simulation. Next, we

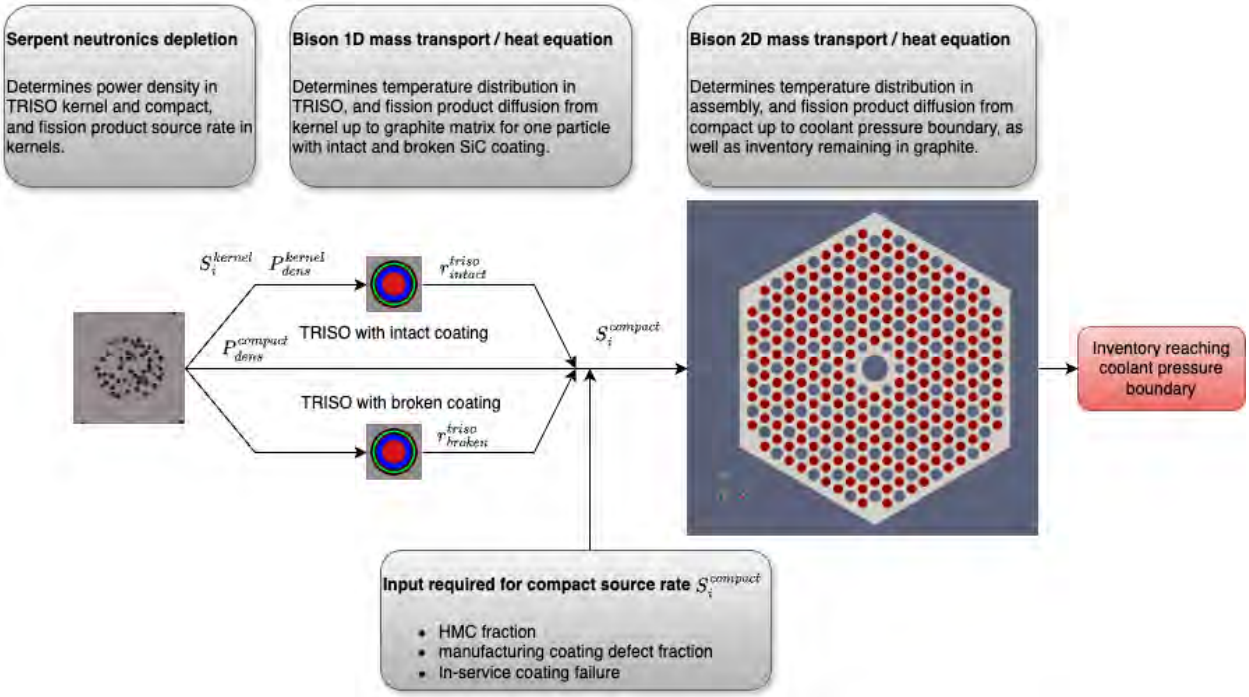
describe techniques for radiation transport leveraging both meshed and meshless techniques for data transfer to multiphysics applications. libMesh adaptive mesh refinement is integrated with OpenMC's tally system, with new techniques to balance runtime, statistical error, and memory usage. This new capability in Cardinal will be demonstrated for a number of nuclear fission applications. Finally, polygon functional expansion tallies (FETs) have been added to OpenMC and will be showcased for data transfers in multiphysics simulation with MOOSE. Crosscutting all these areas, we will describe the verification and validation (V&V) underpinning multiphysics simulation.



Towards a MOOSE-Based Model for Fission Products Transport and Source Term Estimation for High-Temperature Gas-Cooled Reactors

Nicolas Martin (Idaho National Laboratory, INL), Lise Charlot (INL), Gerhard Strydom (INL)

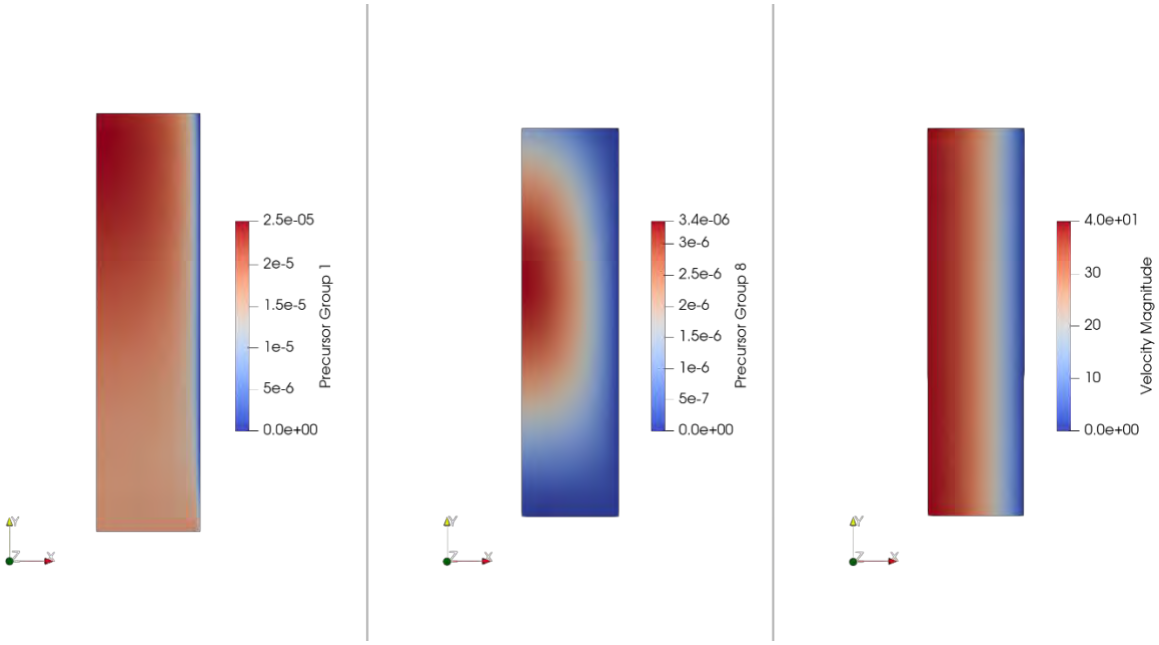
Thanks to fuel elements containing tristructural isotropic (TRISO) particles combined with a low core power density and passive feedback mechanisms leading to modest temperature rises in the event of accidental events, high-temperature gas-cooled reactors (HTGRs) offer a high degree of reliability in terms of fission product retention. While the anticipated source term for HTGRs is expected to be very low, it is important to provide a quantitative estimate of radiological releases during nominal and accidental conditions. We propose a computationally efficient mechanistic source term methodology relying on the Multiphysics Object Oriented Simulation Environment (MOOSE) for tracking fission product transport from TRISO particles up to the coolant pressure boundary, as well as modeling the transport and potential deposition of these nuclides inside the reactor coolant loop. The proposed computational scheme is applied to estimate source term inventories for a representative 10 MWTh prismatic high-temperature microreactor and is qualitatively compared against known release fractions. In addition to providing an alternate analysis tool, this MOOSE model can help reactor designers quantify the influence of key design parameters relevant for radiological dose consequences studies.



Fast molten salt reactor modeling with Moltres

Kyra Lawson (University of Tennessee, Knoxville), Nicholas R. Brown (University of Tennessee, Knoxville)

Molten salt reactors (MSRs) are a type of advanced reactor in which multiple industry and government bodies recently have shown interest due to attractive characteristics such as high operating temperatures and inherent safety features. Various concepts are in design stages and may be constructed in the next few years. It is important that the general behavior of this type of advanced reactor is understood and well-documented in the literature. Safety analyses will be crucial for future licensing endeavors. Providing open-source models may facilitate increased cooperation and understanding regarding the reactor type. This work will present open-source models of fast-spectrum molten chloride salt reactors. Moltres, a MOOSE-based application, is used to solve multigroup diffusion coupled with precursor drift and heat transfer functions. The work is supported by Monte Carlo simulations in Serpent to calculate multigroup constants, reactivity feedback coefficients, and other neutronic parameters. Results are presented in the form of neutron flux graphs, effective multiplication factors, temperature profiles, and delayed neutron precursor concentration maps. The importance of multiphysics modeling of liquid-fueled MSRs is emphasized; pure-neutronics and coupled physics results are compared. Safety-related parameters are discussed. The capabilities of an open-source, MOOSE-based tool are demonstrated, and reproducible models of a fast molten salt reactor concept are provided and analyzed.



RENEWABLES | STORAGE

Dendrite Inhibition using Heteroepitaxial Residual Stress in Zn Metal Batteries

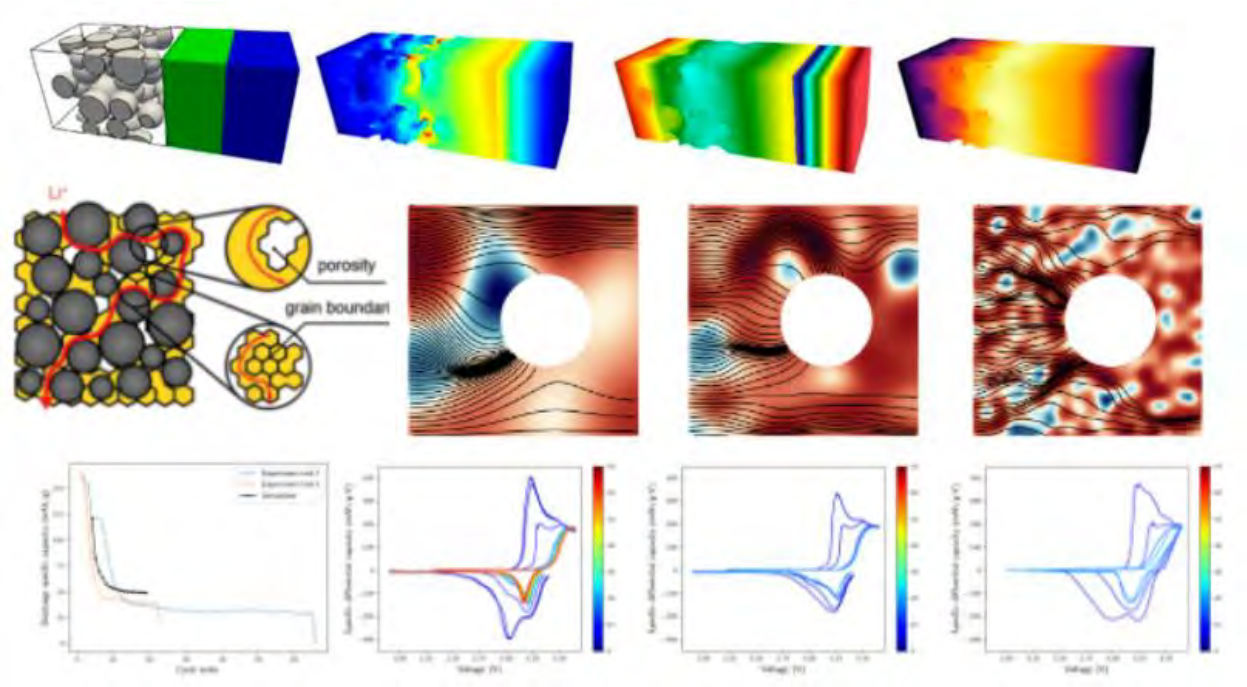
Musanna Galib (The University of British Columbia, UBC), Jian Liu (UBC), Mauricio Ponga (UBC)

Dendrite formation is a long-standing problem for the commercial application of rechargeable metal anode batteries. The well-controlled coating on anodes can solve the problem of instability and uncontrolled reactions between electrodes and electrolytes. Understanding the effects of pre-stressed (residual stress) electrodes with artificial solid-electrolyte inter-phase layer (thin film) on dendrite formation is crucial for the successful application of stable anodes. In this work, using DFT-informed continuum modeling and phase-field modeling, we studied the impacts of residual stresses on the surface evolution of atomic/molecular layer deposited (ALD/MLD) Al2O3 and alucone coating on Zn anodes. During the thin film deposition process, the induced stress arises from two sources, namely, the residual stress during fabrication and the mechanical stress associated with the volume expansion. Of the two, residual stress has largely been considered to have a negligible effect without any rigorous evidence being put forward. Epitaxial stresses are one of the major sources of residual stress in the hetero-epitaxial thin films, which are sensitive to the misfit in crystal lattices existing between film and substrate. The epitaxial stresses influence defect formation in most thin-film systems. We critically assessed alucone and alumina-coated Zn surfaces to depict a prospective methodology to reduce the dendrite growth using the developed hetero-epitaxial residual stress. We used DFT-informed misfit strain analysis in the phase field model to understand the significant consequences of residual stress, such as microstructural changes and deformation in the materials.

A Three-Dimensional, Thermodynamically and Variationally Consistent, Fully Coupled, Electro-Chemo-Thermo-Mechanical Model of Solid-State Batteries

Tianchen (Gary) Hu (Argonne National Laboratory, ANL), Bipul Barua (ANL) Mark Messner (ANL)

We will present a tool for three dimensional, high fidelity, coupled electro-chemo-thermo-mechanical modeling of solid-state batteries. A complete version of the tool is available as open source software at https://github.com/hugary1995/eel.git. The theoretical framework of the tool revolves around an inf-sup statement on a total potential, comprising the Helmholtz free energy, the electrical kinetic potential, the chemical potential, the Fourier potential, the chemical reaction potential, and the external power expenditure. The tool uses MOOSE and a variational formulation to solve the boundary value problem for solid-state battery incorporating the full set of multiphysics couplings. The variational formulation also enables a modular software architecture for the tool so additional physics can be easily included by specifying the new contribution to the total potential. We will present several implementational details and example problems. Finally, simulation results from complete charge/discharge cycles of a solid-state battery will be shown.

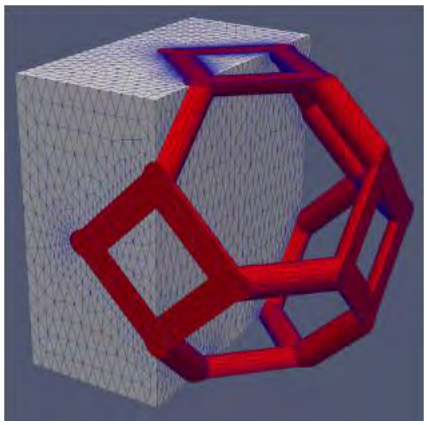


Parameterizing the influence of moisture on the thermal performance of TES

Abhishek Bhesania (Argonne National Laboratory, ANL)

Thermal Energy Storage (TES) systems play a crucial role in renewable energy grids by storing surplus energy during the day and releasing it when demand is high or during nighttime. Magnesium chloride (MgCl2) is a promising phase-change material (PCM) for TES due to its high energy density and high melting point (>700Â°C). To improve the heat transfer in TES, PCM is often impregnated within a porous matrix of high thermal conductivity materials, such as graphite. However, moisture infiltration presents a significant challenge in TES facilities, potentially altering the PCM's integrity. Moisture can trigger hydrolysis reactions, releasing chlorine, which may corrode metal storage

containers. Corrosion byproducts can mix with PCM and alter its composition and properties. Due to its hygroscopic nature, MgCl2 readily absorbs moisture, changing its hydrous state and modifying its bulk properties. In this study heat transfer simulations are performed to investigate the influence of moisture on TES system performance. A mesoscale representative model of graphite foam impregnated with MgCl2 in various hydrous states is developed. Using the Asymptotic expansion homogenization technique, we derive effective anisotropic thermal properties for a range of temperatures relevant to TES operations, using the single-phase properties of individual components as inputs. These derived properties are integrated into larger-scale heat transfer simulations of the TES system to assess its performance. The system-level model not only quantifies moisture's effect on TES performance but also provides essential inputs for degradation models at lower scales, establishing a comprehensive understanding of moisture-induced performance variations in TES. We perform a parametric study by varying certain key operating parameters of the TES systems working with different MgCl2 hydrates. A surrogate model is trained on the thermal performance data obtained from the parametric study and presented at the end.

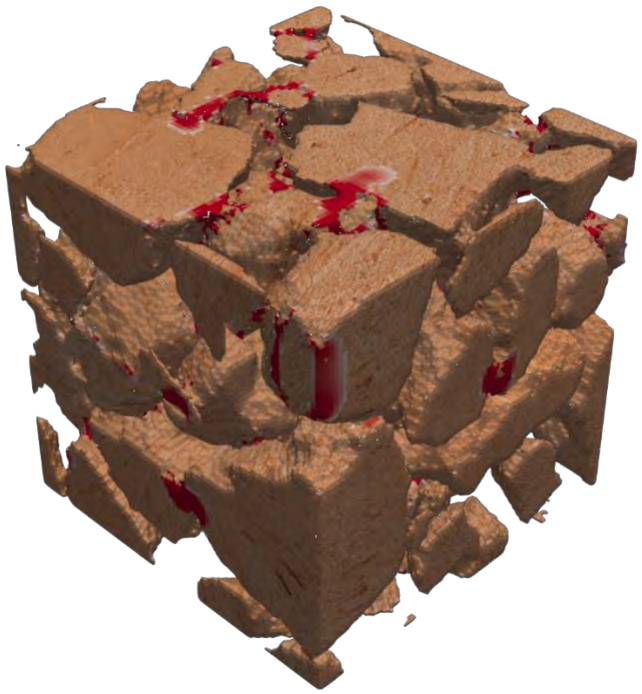


Studying Cyclic H2 Injection in Underground Storage Using a Digital Rock Physics Framework

Sijmen Zwarts (TU Delft), M. Lesueur (TU Delft)

H2 is a promising clean and renewable energy source, especially when produced using green energy without CO2 emissions. However, due to H2's low energy density (over five times lower than CH4) it requires significantly larger storage volumes. As a result, underground storage, such as depleted oil or gas reservoirs, are being explored as potential solutions for underground H2 storage (UHS). The cyclic nature of green H2 production leads to repeated injection and extraction cycles, which in turn subject the rock formations in UHS to cyclic loads. The mechanical response of the rock to cyclic loading is critical for the long-term stability, safety, and efficiency of UHS operations. Laboratory experiments typically show that mechanical response of the rock under cyclic loading evolves through three stages under cyclic loading. Initially, a rapid increase of the irreversible strain is observed during the first cycles. This is followed by a stabilization of the additional irreversible strain per cycle, either in a linear trend or through complete stabilization. Finally, an acceleration of the irreversible strain is observed, leading to the failure of the rock. The rock microstructure and the

effect of the load cycles will determine the evolution of the mechanical properties over time. In addition to the general evolution of irreversible strain, research also shows that in perfect elasticity, there is no irreversible strain accumulation over the cycles. However, when the sample is loaded above a certain stress point below the yield point, an accumulation of irreversible strain is still observed. To understand the mechanical behaviour of rocks under cyclic loading, our simulations focus on replicating cyclic experiments, for which CT-scans have been obtained. These images are the basis of our Digital Rock Physics framework for which Finite Element simulations of mechanics are run on a 3D mesh of the microstructure reconstructed with the ImageFunction of MOOSE. Upscaling of the microscale model allows to retrieve unique macroscopic behaviour. The simulator is based on the developments of the REDBACK application. We emphasise on separating the microstructural phases (grains, voids and clay bonds) each contributing to different macroscopic behaviour. By implementing inherent elasto-viscoplasticity of clay, which allows the material to accumulate irreversible strain in overstress, we capture the accumulation of irreversible strain per cycle. We find a natural transition from the initial rapid increase of irreversible strain to a stabilization of the latter due to pore collapse of the granular medium. Additionally, we capture strain accumulation before the macroscopic yield point, where micro-strains at the lower scale gradually build up, contributing to the irreversible strain. Future work will focus on the final stage and grain interactions will also be investigated.

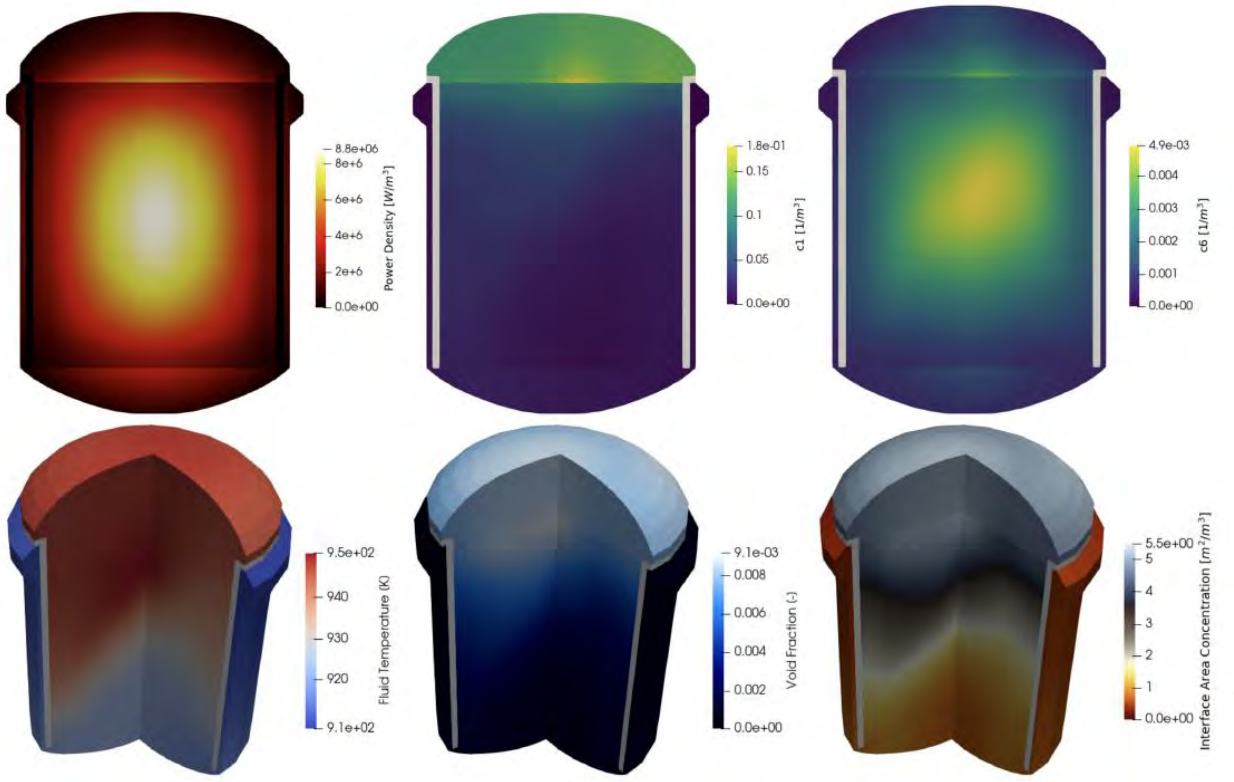


FRAMEWORK 1

Overview of thermal-hydraulics capabilities in MOOSE for nuclear reactor modeling

Mauricio Tano (Idaho National Laboratory, INL), Peter German (INL), Ramiro Freile (INL), Mengnan Li (INL)

The Navier-Stokes module in the MOOSE framework has been significantly enhanced since 2021 through the adoption of the finite volume method. This advancement has resulted in a more robust tool capable of performing multi-fidelity Computational Fluid Dynamics (CFD) analyses. This paper presents the latest developments integrated into the Navier-Stokes module of MOOSE, focusing on the implementation of advanced two-equation turbulence models, the enhancement of multi-dimensional two-phase flow models, and the improvement of numerical methods employed in the solver. The two-equation turbulence models, specifically the k-epsilon and k-omega-SST models, have been incorporated into the MOOSE Navier-Stokes module. These models include the standard formulations and various corrections to account for non-equilibrium wall functions, low Reynolds number effects, curvature, and vortex stretching. Detailed descriptions of these turbulence models are provided, along with the validation cases employed to verify their accuracy and reliability. The implementation of these turbulence models enhances the module's capability to simulate complex turbulent flows with higher fidelity. In terms of two-phase flow modeling, a significant development is the implementation of a multi-dimensional generalization of the drift-flux mixture model. This model resolves the transport of a liquid-gas mixture, incorporating specific correlations for the slip velocity between the gas and liquid phases. The presentation provides a comprehensive description of the drift-flux mixture model, and the validation cases used to assess its performance. The implementation of this model addresses the need for accurate simulation of multi-phase flow scenarios, which are crucial in various engineering applications, including nuclear reactor safety analysis and chemical process engineering. Furthermore, two notable numerical advancements have been recently integrated into the Navier-Stokes module of MOOSE. First, the capability to compute gradients using the least-squares method has been introduced. This approach is particularly beneficial when dealing with skewed meshes, as will be demonstrated in the example problem of a fluoride-cooled pebble bed reactor. The least-squares gradient computation enhances the accuracy of the numerical solution in such challenging mesh configurations. Second, the implementation of second-order limiters has been achieved. These limiters are crucial for maintaining solution accuracy while preventing numerical oscillations in high-gradient regions. The impact of the limiter system is showcased through the forced convection operation of an open-source model of the Molten Chloride Reactor Experiment. This example illustrates the effectiveness of the limiters in preserving solution quality and stability in simulations involving steep gradients.



Enhancement of System Thermal-Hydraulics Simulations Using Block-Dependent and Time-Dependent Scaling Factors: Development and Implementation in the SAM Code

Eric Cervi (Argonne National Laboratory, ANL)

SAM is an advanced and modern system analysis tool under development for transient safety analysis of various advanced non-light water reactors, under the U.S. DOE Office of Nuclear Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. SAM strives for advancements in physical modeling, numerical methods, and software engineering to enhance its user experience and capability for reactor transient analyses. It utilizes the MOOSE framework to leverage modern software environments and numerical methods. Proper scaling of equations is critical in solving nonlinear systems of equations because they impact the accuracy, convergence, and stability of numerical methods. In SAM system thermal-hydraulics simulations, scaling presents significant challenges across various situations due to dynamic change of scaling with time, space, and across different physics. In transient simulations, flow conditions can change drastically over time. For example, strong velocity changes may occur due to pump trips, valve operations, or the initiation of natural circulation. Additionally, flow rates can vary significantly across the computational domain for example, high flow rates in primary coolant loops compared to stagnant or slow-moving regions in bypass channels. Such disparities can result in poor scaling of the momentum equation, as scaling factors based on global averages often fail to account for local conditions. To address these challenges, physics-informed block (spatial)-dependent and time-dependent scaling factors were developed and implemented in the SAM code. This new capability supports both 1D fluid channels and heat conduction in solid structures. By

leveraging this feature, proper scaling factors can be computed for each domain based on local flow conditions, thereby improving the local scaling of the balance equations. Additionally, these scaling factors are updated dynamically over time to account for variations in flow conditions during transient simulations. The new capability was assessed using several test cases involving different power plant components, including coolant channels and thermally coupled solid structures. Compared to constant, uniform, user-defined scaling factors, this new approach effectively scales equations over a wide range of operating conditions. Consequently, users no longer need to search for these factors manually. Since the scaling factors depend on local flow conditions, the new approach can account for situations in which the flow conditions change over time or exhibit strong spatial variations across the domain.

The Functor system: a new on-the-fly take on Material Properties based on C++ functions

Guillaume Giudicelli (Idaho National Laboratory, INL), Alexander Lindsay (INL)

In the context of solving multiphysics problems, the discretization of the partial differential equations (PDE) at hand often takes the spotlight. However, for most engineering users and even application developers, the discretization of the equations has already been performed. Instead, they are tasked with implementing specific closure relations and material properties. MOOSE has long enabled this using the Materials system. This system relied on the pre-computation of all properties before they are used in the PDE or in postprocessing. In this talk we will introduce the Functor system, which was deployed in MOOSE in 2021, then present a few applications of functors in flow modeling simulations by the NEAMS program. Functors first offer great flexibility in their evaluation. Rather than storing various arrays for material properties, they are evaluated on the fly at the location and state, e.g. current or old value, requested. Unlike regular material properties, several operations such as the time derivative, the divergence and the curl can be requested from a functor. Similar to material properties, functors can be made to depend on arbitrary combinations of variables, functions, postprocessors and other properties. However, unlike material properties, any of these can be substituted for a functor material property. Thanks to this, objects no longer need to be duplicated based on the types of their parameters.

Coupling of Scalar and Field Variables in MOOSE Using the Scalar Augmentation Class System

Timothy Truster (University of Tennessee, Knoxville, UTK)

Recently, a "Scalar Augmentation Class" system was implemented in the MOOSE framework to facilitate coupling of scalar and field variables for a broad class of problems. Previously existing architecture in the code required the user to develop a UserObject to perform the assembly loop of the quantities for the scalar variable, and lower-level API assembly calls were required for the off-diagonal coupling terms between the field and the scalar variable. While user objects are general and might provide better parallel speedup by minimizing access to global matrices, they are more difficult for the user to program. Thus, the goal of this contribution is to provide standard methods for assembling scalar variable contributions for coupling within Kernel and MortarConstraint

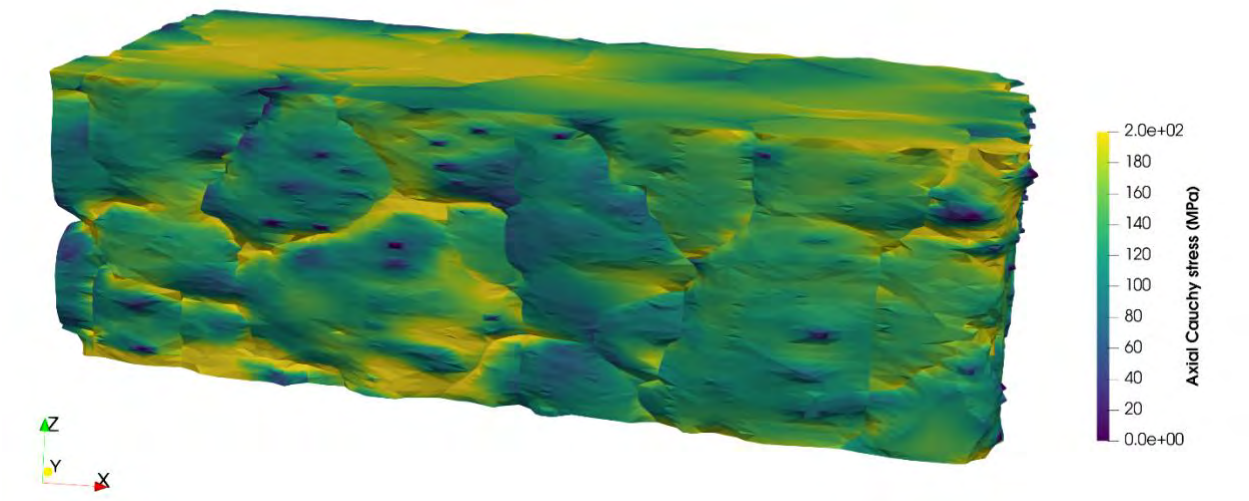
objects. This goal is realized by adding derived classes onto the base kernel and mortar constraint classes and providing methods with pre-built quadrature loops and assembly method calls for each of the possible combinations of field and scalar variables associated with the object. This development enables formulations such as periodic boundary conditions to be handled weakly on nonconforming meshes through surface integrals rather than volume integrals. Examples provided in the MOOSE framework will be presented to showcase the features of the augmentation class, mostly associated with solid mechanics applications. Lastly, related developments on interface kernels and Discontinuous Galerkin objects within our group's application BEAVER will also be highlighted.

SPECIAL TOPICS 1

New crystal plasticity capabilities in MOOSE/NEML2

Mark Messner (Argonne National Laboratory, ANL), Gary Hu (ANL)

MOOSE has long supported crystal plasticity finite element simulations for microscale material behavior. However, recent developments in the MOOSE framework and the solid mechanics module aim to improve the numerical performance of simulations of this type. Discretizing reasonably representative volumes of material requires large scale simulations with millions of elements to capture local variations in the material microstructure. The resulting simulations can be difficult to solve effectively on HPC systems as (1) the discretized field problem for stress equilibrium is typically highly nonlinear and it can be difficult to effectively scale the solution of resulting linearized system of equations with AMG techniques (2) often periodic boundary conditions and homogenization constraints are applied to the simulation, which can degrade the conditioning of the linearized system of equations and further reduce the effectiveness of the linear solver, and (3) the simulations have a different balance of work compared to macroscale solid mechanics models, where evaluating the complex local single material model often consumes a significant amount of the solution time, compared to the global solve. This talk discusses these challenges in the context of several actual example and provides suggestions for how to mitigate them in MOOSE simulations. This includes examples using the new NEML2 GPU-enabled material model solver now packaged with the solid mechanics module to speed up the material model evaluation on hybrid machines and a brief discussion of some of the features of the single crystal modeling framework in NEML2.



Modeling of Liquid Infiltration in Powder Processing Manufacturing Techniques

Huy Tran (Argonne National Laboratory, ANL), Tianchen Hu (ANL)

The infiltration of liquid material into porous structures is one of the most economical powder processing techniques that enhances the final product's durability and performance in many advanced manufacturing processes. However, under-infiltration, reaction, as well as non-optimal infiltration and cooling rates, could cause high residual stress, leading to excessive distortion and premature fracture. These effects, being multiscale by nature, are not well understood despite decades of development. In this work, we developed a Multiphysics model in MOOSE, as part of the MOOSE-based Powder Utilization Modeling Application (PUMA), to simulate the infiltration process inside a porous medium. The model couples the diffusion-reaction to the heat and momentum balance equation to govern the macroscopic infiltration behavior, as well as the resulting temperature, displacement, and stress. We track the composition and porosity evolution depending on the macroscopic saturation of the infiltrated liquid, which in turn, provides the diffusivity, heat capacity, reaction, and expansion rate back to the macroscopic governing equations. We apply this model for liquid silicon infiltration (LSI) into porous C/SiC composites, manufactured through powder processing. Results of the fully coupled simulations will be shown which provide key insight into optimal manufacturing parameters.

A Numerical Study on Adaptive Printing Velocity Control in Frontal Polymerization-Assisted Thermoset Polymer 3D Printing

Xiang Zhang (University of Wyoming, UW), Zhuoting Chen (UW), Chao Jiang (UW)

A revolutionary curing technique known as frontal polymerization (FP) has emerged for rapid and energy efficient thermoset polymer and polymer composite manufacturing. FP harnesses a self-propagating exothermic reaction front to swiftly polymerize thermoset monomer resins, showcasing notable energy efficiency and expedited production of fully cured thermosets. This

advancement has spurred the exploration of various engineering applications, particularly in the realm of 3D printing. While existing research underscores successful fabrication endeavors employing FP-based 3D printing, a primary hurdle lies in optimizing printing process parameters, which currently necessitate iterative experimentation. This bottleneck impedes the broader adoption and scalability of FP-based 3D printing for practical applications. In our prior work, we developed a multiphysics modeling framework for FP-based 3D printing processes within the Multiphysics Object-Oriented Simulation Environment (MOOSE) [1]. This framework integrates coupled thermos-chemical processes with element activation for ink deposition. Through experimental validation, we revealed the intricate interplay between printing velocity, printing length, front behavior, temperature distribution, and polymerization processes. One of the key factors for successful printing is to ensure the polymerization front to follow the extusion nozzle closely. Nevertheless, maintaining a delicate balance between the front and nozzle proves challenging during constant velocity printing, potentially leading to filament deformation. In this presentation, we introduce a closed-loop control simulation system aimed at adaptively adjusting printing velocity during the printing process to ensure that the nozzle-to-front distance remains within predefined tolerances, thereby mitigating ink deformation before curing. The simulation commences with an initial printing velocity and runs for a designated time interval, Î”t, akin to the sensing interval in experimental setups. Subsequently, the simulation pauses, and results are analyzed to compute the nozzle-to-front distance, dictating the maximum allowable printing velocity for the next time interval. This iterative process continues until printing concludes. Leveraging this numerical closed-loop control system, we scrutinize the effects of variable printing velocity on printing processes and resultant part quality in a layer-by-layer printing paradigm. We focus on understanding the adaptive frontal velocity control on the printing process and the printed part qualities, providing guidance for future experiment experimental development. Reference [1] Z. Chen, M. Ziaee, M. Yourdkhani, X. Zhang, Multiphysics modeling of frontal polymerization-assisted layer-by-layer additive manufacturing of thermoset polymer components, Addit. Manuf. 59 (2022) 103182.

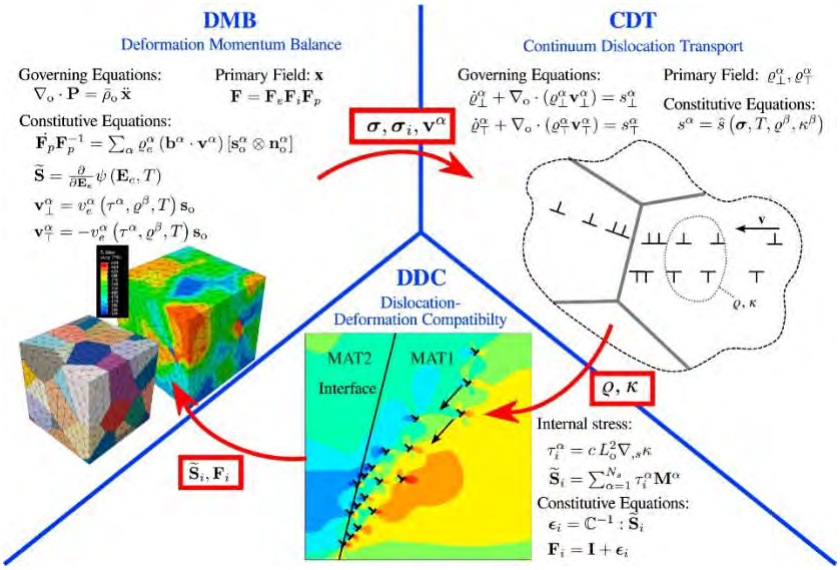
NUCLEAR 2

A Dislocation Transport based Crystal Plasticity model to study Structure-Property relations in Polycrystalline Materials

Brayan Murgas (Los Alamos National Laboratory, LANL), Subhendu Chakraborty (LANL), Abigail Hunter (LANL), Darby Jon Luscher (LANL)

In the present work, we develop a novel dislocation density-based crystal plasticity (CP) model by extending the transport-based CP model “Discoflux” [1] to understand and predict the effect of the underlying microstructure on the mechanical properties of the polycrystalline metallic materials. The special feature of this CP model is that the evolution of dislocation density has both local as well as non-local contributions. The local contribution involves dislocation nucleation, annihilation, multiplication, and trapping. The non-local contribution originates due to dislocation transport within the grain and across grain boundaries. Dislocation transport within the grain is modelled by solving standard field advection equations, while dislocation transfer across a GB is modelled using an interface “advective flux transfer” model. We also extend a geometric criterion

to determine the preferred slip systems involved in dislocation transfer across the GB. This criterion consists of five geometric quantities (slip plane normal and slip direction in each grain and grain boundary plane normal) and two material parameters (critical dislocation density and critical resolved shear stress at the GB). The complete model is implemented within the open-source code MOOSE. We apply this model to study the effect of grain misorientation on the mechanical properties of pure Copper and compare the result with the bi-crystal and polycrystal experimental observation of the same material. [1] D. J. Luscher, J. R. Mayeur, H. M. Mourad, A. Hunter and M. A. Kenamond, IJP, 76 (2016) 111-129

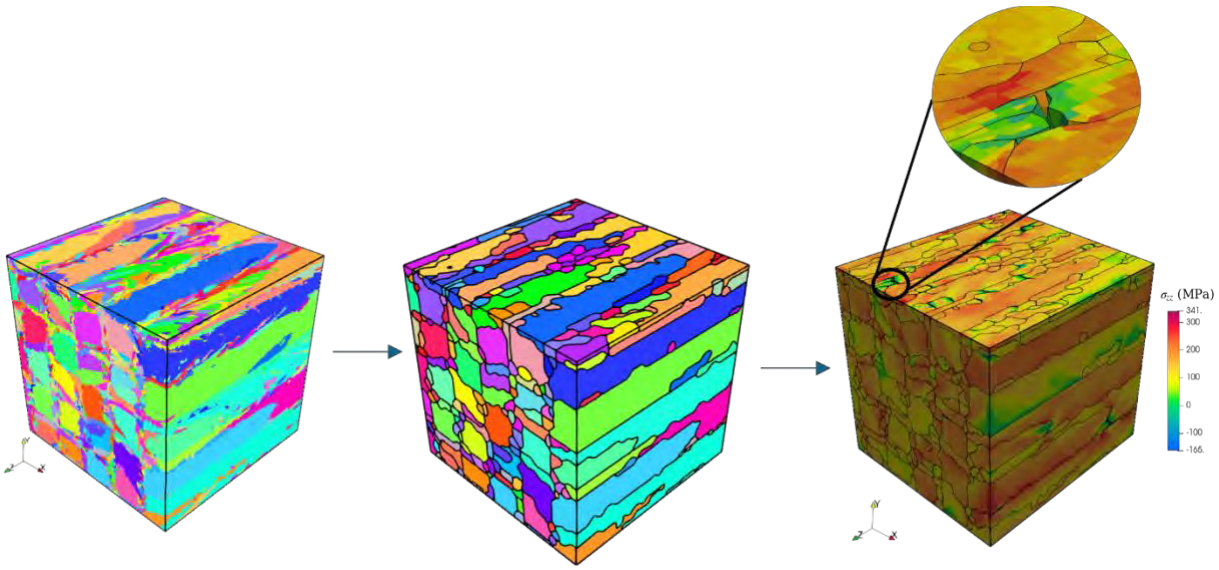


Modeling the impact of morphological features of complex microstructures using MOOSE based Crystal Plasticity Finite Element Model

Sagar Bhatt (Argonne National Laboratory), Mark C. Messner (ANL)

Advanced manufacturing techniques like diffusion bonding and laser powder bed fusion have enabled development of complex geometries leading to more efficient components such as compact heat exchangers, proposed to be used in upcoming advanced nuclear reactors and concentrating solar power plants. Deploying these components under such harsh service conditions requires a thorough understanding of their long-term performance, particularly the influence of unique microstructural features resulting from these new manufacturing methods. In the absence of long-term creep test data, predictive modeling techniques, specifically finite element methods, have become essential for understanding the microstructure-property relationships in these materials. We generate high-fidelity finite element meshes that represent the complex microstructures using three-dimensional data obtained from phase-field simulations, cellular automata, and Monte Carlo grain growth simulations. The sub-structural features, such as unrecrystallized boundaries in diffusion bonded microstructures, are incorporated in the mesh using MOOSE's mesh generator tools. Creep deformation itself is modeled using a MOOSE-based crystal plasticity finite element framework, DEER, which uses constitutive material models

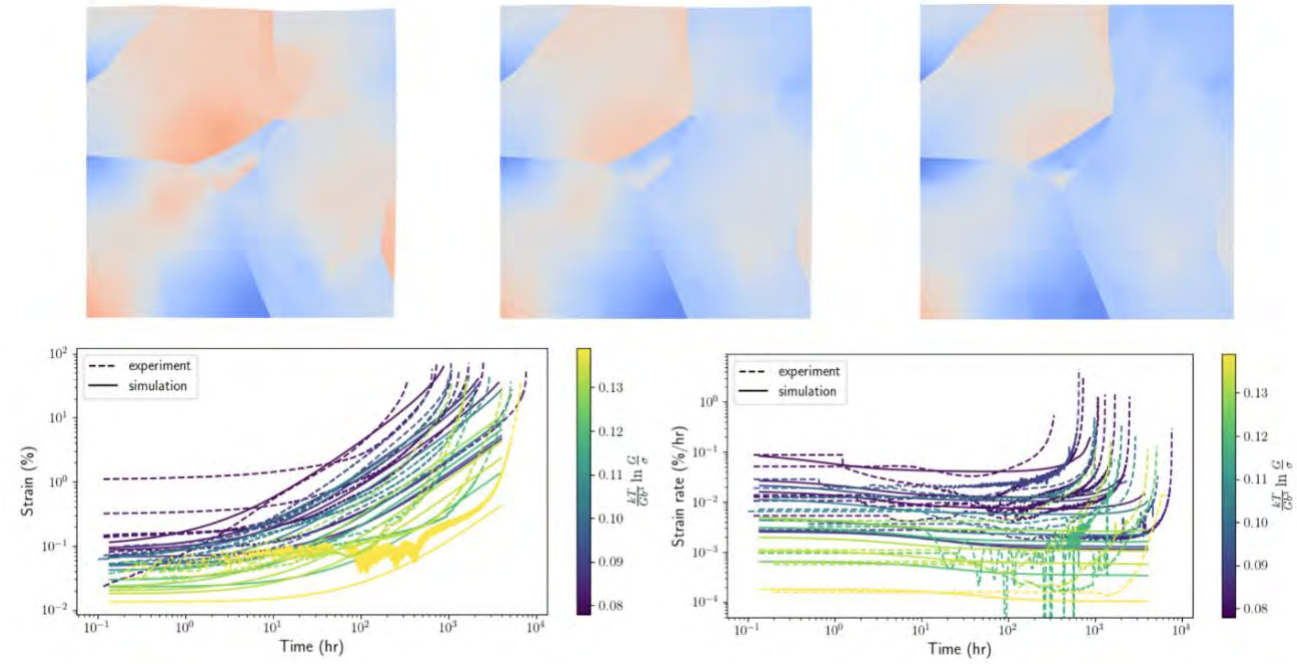
implemented in the material modeling library NEML. In this work we will present some of our modeling techniques and results that can help understand the impact of these complex microstructural features on the performance of the material.



Mechanistics Model for Predicting Uniaxial Creep, Multiaxial Creep, and Stress Relaxation Behavior of Alloy 709

Shahmeer Baweja (Argonne National Laboratory, ANL), Tianchen (Gary) Hu (Argonne National Laboratory, ANL)

A physics-based model has been developed to predict uniaxial and multiaxial creep, as well as long-term stress relaxation behavior, in Alloy 709, an advanced austenitic steel intended for high-temperature applications like Sodium Fast Reactors (SFRs). Alloy 709 surpasses conventional stainless steels like 316 and 304 in high-temperature resilience, yet it lacks extensive data on creep and stress relaxation. This model leverages a crystal plasticity finite element (CPFE) framework to simulate the material's deformation and failure mechanisms, incorporating an extended Hu-Cocks dislocation creep approach with precipitation effects and a Sham-Needleman model for grain boundary cavitation-induced failure. Stability is improved through a novel update algorithm, and a surrogate model trained on CPFE simulations accelerates forward evaluations. Stochastic variational inference (SVI) refines microstructural parameters, enabling the calibrated model to provide reliable, long-term predictions, benchmarked against empirical methods, to support faster qualification of Alloy 709. The model also provides insights into key questions surrounding stress relaxation behavior, such as threshold stress, strain thresholds for damage initiation, damage accumulation dynamics, failure likelihood, and the applicability of engineering models for relaxation damage.

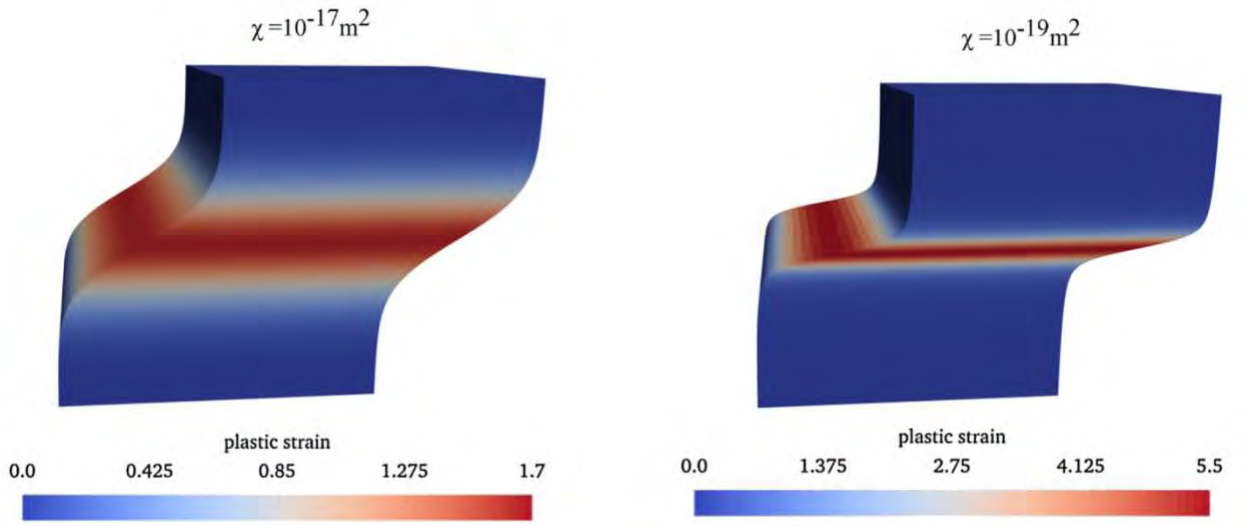


GEOSCIENCE 1

Multiphysical Couplings and Cosserat Continua to Model the Localization of Deformation in a Fault Core

Hadrien Rattez (UCLouvain), Ioannis Stefanou (Ecole Centrale Nantes), Thomas Poulet (CSIRO), Manolis Veveakis (Duke University), Jean Sulem (Ecole des Ponts ParisTech)

Induced seismicity is major hazard associated with the injection of a fluid underground, as it is done for deep geothermal or H2/CO2 storage projects. In this contribution, we aim at understanding the mechanisms involved in a fault during a seismic slip. Those unstable slips in the brittle part of the lithosphere are often accompanied by extreme shear strain localization into a narrow, thin zone, which is called Principal Slip Zone (PSZ). According to field observations, the PSZ has a finite thickness and varies from hundreds of microns to few centimeters. The size of this zone plays a major role in the mechanism of earthquakes as it affects the energy budget of the fault core and its stability. We model here the creation of shear bands inside a fault zone considering the effect of microstructure by resorting to elastoplastic Cosserat continua and Thermo-Hydro-Chemo-Mechanical couplings. The use of Cosserat theory not only enables to regularize the problem of strain localization by introducing an internal length into the constitutive equations, but at the same time it introduces information about the size of the microstructure. The results obtained with numerical simulations performed in the application Redback are compared with experimental and in situ observations for the shear band thickness and the fracture energy. It enables us to understand the role of various phenomena on the behavior of a fault, such as thermal pressurization or the size of the microstructure, among others on the thickness of the band but also on the stability of the system.



A Coupled Discontinuous Galerkin and Cohesive Zone Implementation for Modeling Hydraulic Fractures in Porous Media

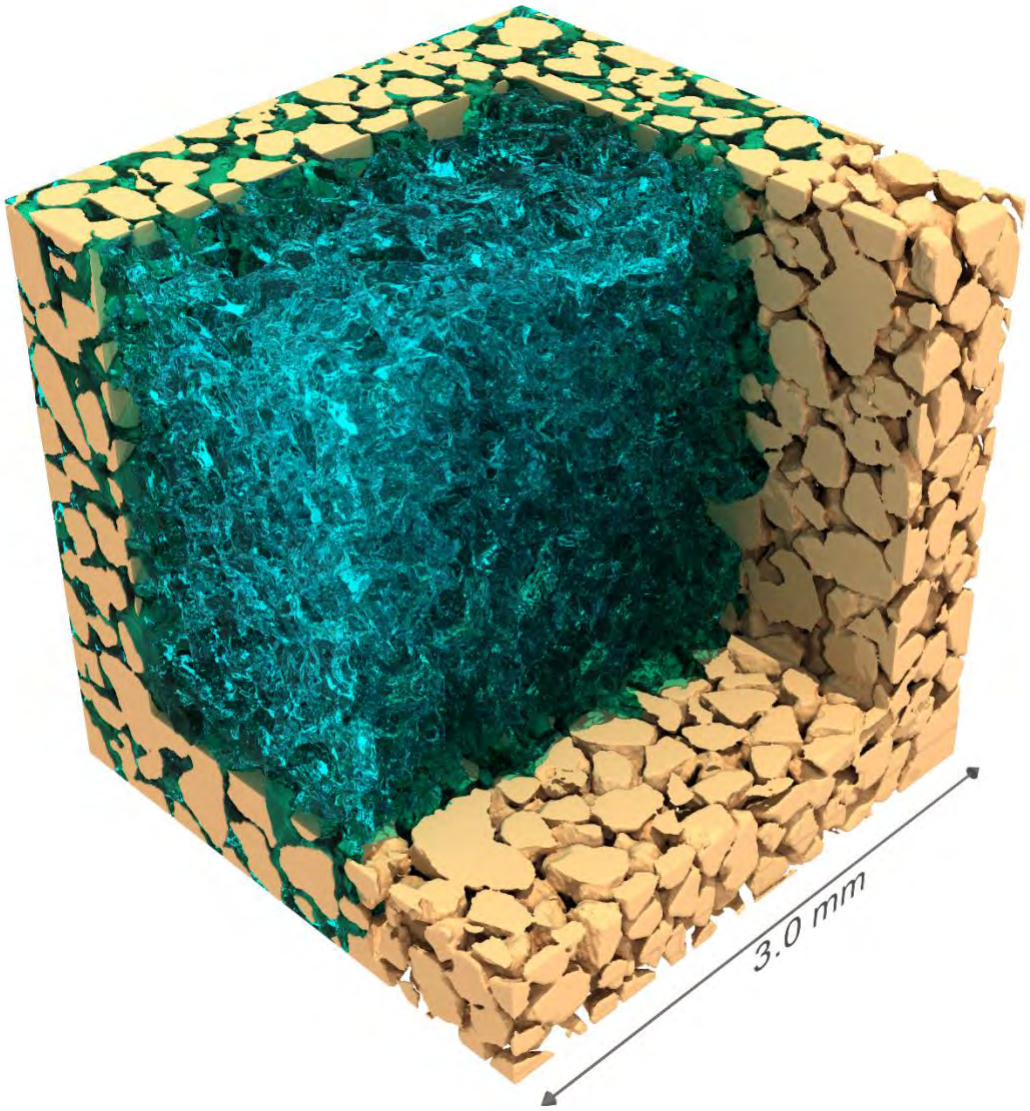
Ming Yang (Idaho National Laboratory, INL), Wencheng Jin (Texas A&M University), Ruijie Liu (INL), Robert Podgorney (INL)

Hydraulic fracturing is a widely practiced stimulation technique to enhance the formation permeability in unconventional oil & gas and geothermal reservoirs. However, modeling hydraulic fracturing poses significant computational challenges, such as simulating fracture propagation, rapid fluid flow within narrow fractures, abrupt fluid pressure variations along fracture walls, and the interaction between solid and fluid phases. In this work, we introduce a lower-dimensional interface element, formulated using the discontinuous Galerkin (DG) finite element method, to explicitly represent potential crack surfaces. Fracture initiation and propagation are governed by embedded cohesive zone models, while fluid flow within the crack aperture is simplified by averaging quantities along the aperture, enabling fluid coupling within the interface element. This numerical formulation has been implemented in ELK (ELectric fracKing), a MOOSE-based finite element application designed to simulate fracture propagation in porous media. The methodology was verified against benchmark examples, including KGD & PKN hydraulic fractures. Furthermore, we applied this framework to investigate 1) the simultaneous propagation of multiple closely spaced fractures in a homogeneous formation and 2) a single hydraulic fracture propagation in a multilayer formation with heterogeneous properties. Parametric study on fluid viscosity, rock toughness, in situ stress anisotropy, and fracture spacing will be reported.

Three-Scale Multiphysics Framework Modelling Fault Reactivation

Martin Lesueur (Delft University of Technology), Manolis Veveakis (Duke University), Thomas Poulet (CSIRO)

Induced seismicity happens as fluid injection or production alters the in-situ stress field, eventually reactivating nearby dormant faults. Such event can have both operational and environmental catastrophic consequences and needs therefore to be prevented at all costs. In deep carbonate reservoirs, the fault reactivation is often accompanied with a large increase of permeability due to the dissolution of the rock, leading additionally to unwanted pressure equilibration in an initially compartmentalised reservoir. A multiscale multiphysics computational framework is introduced in REDBACK, a MOOSE application, to model this complex thermo-hydro-mechanical-chemical fault behaviour. The framework incorporates two layers of Multiapps as a three-scale approach: (a) at the reservoir scale (kilometers), poromechanics govern the bulk reservoir response, while faults are treated as frictional lower-dimensional interfaces; (b) at the fault meso-scale (meters), a thermo-poro-chemo-visco-elasto-plastic model simulates fault reactivation dynamics, including shear heating and chemical dissolution; (c) at the micro-scale (micrometers), meso-scale properties such as permeability are upscaled from Stokes flow simulations on digital rocks, accounting for chemo-mechanical alterations of the fault's pore structure. The Digital Rock Physics framework at the micro-scale is based on the ImageFunction to mesh rock microstructures from ÂµCT-scans. Dissolution/precipitation cycles are implemented with an ElementSubdomainModifier and can retrieve permeability hysteresis. Unlike traditional models relying on empirical laws, this framework dynamically upscales physical laws, offering continuous transitions between fault activation, evolution, and deactivation phases. The results demonstrate the importance of fault microstructure and its role in seismicity. Simulations reveal that even subtle variations in microstructural geometry can significantly impact the timing and duration of reactivation events. Our model successfully captures the non-linear, heterogeneous slip propagation and permeability changes observed during fault valve behavior, offering enhanced predictive capabilities for seismic risk assessment in carbonate reservoirs.



SPECIAL TOPICS 2

Coupling MOOSE's Electromagnetic Module and Plasma Fluid Application for the Study of Microwave-Driven Discharges

Corey DeChant (Idaho National Laboratory, INL), Casey Icenhour (INL), Nafisa Tabassum (North Carolina State University, NCSU), Sathya Ganta (Applied Materials Inc., AMI), Kallol Bera (AMI), Abdullah Zafar (AMI), David Peterson (AMI), Steven Shannon (NCSU)

Within the MOOSE (Multiphysics Object-Oriented Simulation Environment) framework, the electromagnetic module and plasma fluid application (Zapdos) were coupled together to study the

transition in microwave driven plasmas from under- to over-dense. A plasma is referred to as under-dense when the electron density is low enough that the electric fields of the microwaves can propagate freely throughout the plasma domain. As the electron density increases, such that the plasma frequency approaches the drive frequency of the system, the plasma transition to a regime commonly referred to as over-dense. Within the over-dense region, the plasma starts to impede the propagation of the electric fields through the plasma. This results in localized power deposition at the edges of the over-dense region. Electric fields were obtained utilizing MOOSE's internal electromagnetic solver, while the plasma dynamics were solved by MOOSE's multi-fluid plasma application, Zapdos. Two-way coupling between the solvers were incorporated to investigate the degree of feedback between the field propagation, power deposition, and plasma parameters (such as electron density, electron temperature, collision frequency, etc.) in 2D axisymmetric simulations. The two main pathways of coupling between the physics domains are the power deposition supplied from the microwaves into the plasma and the dynamic plasma permittivity that influences the propagation of microwaves. Simulation results were compared to experimental measurements for the purpose of validation and correlating changes in the plasma shape seen in experiments to the onset of the over-dense transition determined by simulations. The plasma was driven by supplying a microwave signal (~2.45 GHz) into an axisymmetric applicator above a vacuum chamber, with the power supplied into the applicator ranging between 25 - 125W. For gas chemistry, focus was placed on argon at mid-pressure ranges (~0.2 Torr to a few Torr).

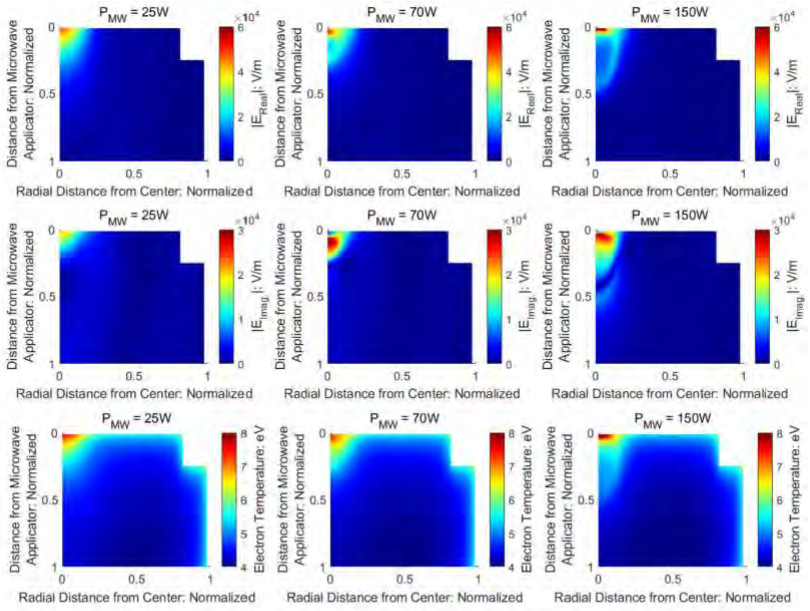
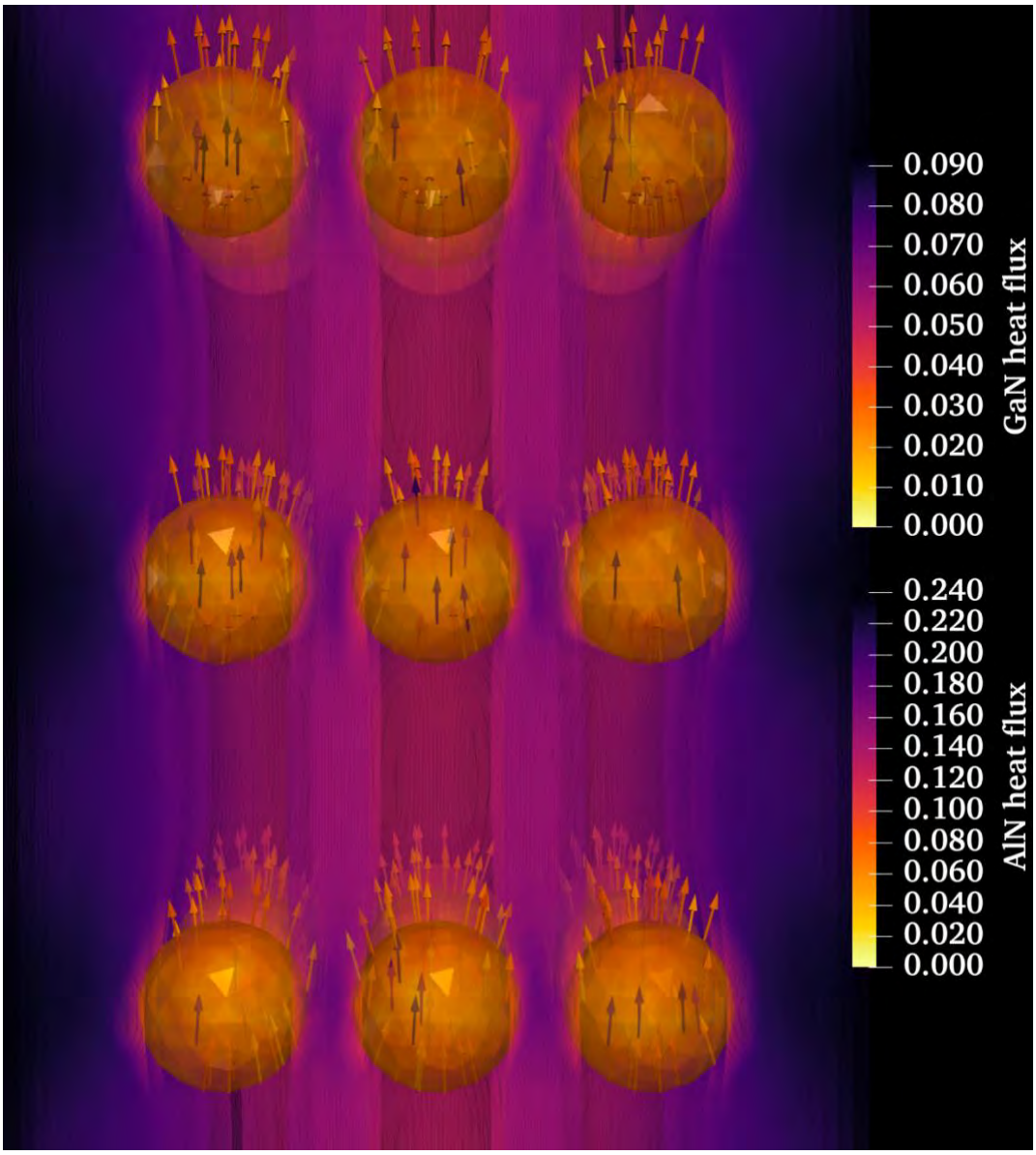


Figure 1: The propagation profiles of the magnitude of the real (Top) and imaginary (Middle) component of the electric field within an argon plasma and the electron temperature profile (Bottom) of the plasma for microwave powers of 25W, 70W, and 150W. The power setting correlate to a fully under-dense plasma, the onset of an over-dense region, and a fully developed over-dense region, respectively.

Modeling Spectral Phonon Transport at Thermal Interfaces in Heterostructures

Jackson Harter (Idaho National Laboratory), Cameron Chevalier (University of California – Riverside, UCR), P. Alex Greaney (UCR)

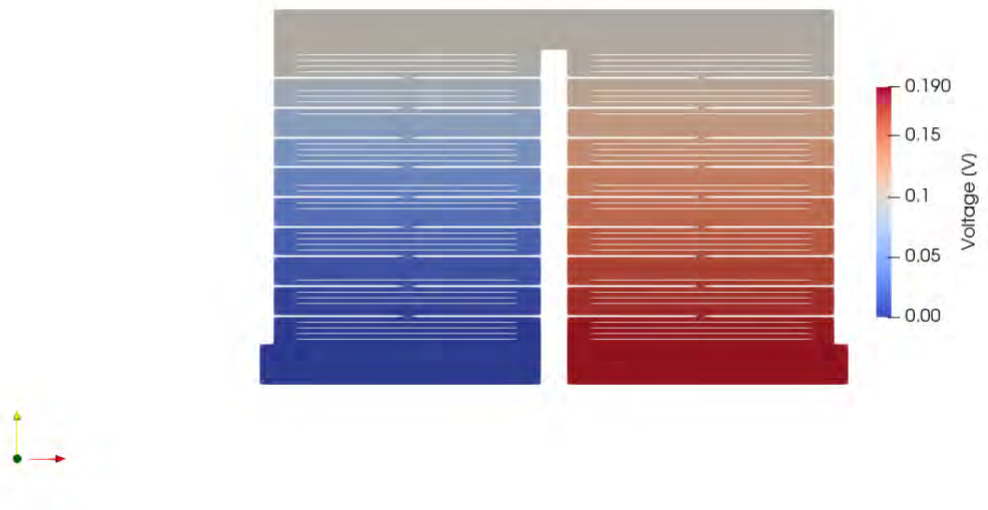
We present a multigroup phonon transport model for calculating the effective thermal conductivity materials with thermal resistance from heat transport across internal interfaces for the efficient prediction of heat flux, temperature distribution, and thermal conductivity in various layered materials. This approach leverages the spectral Boltzmann transport equation for phonons, in the self-adjoint angular flux formulation using discrete ordinates for angular discretization and continuous finite elements for spatial discretization. A closure term acts as a redistribution kernel for the total energy bath in the systems, and is an effective indicator of the degree of disorder between the spectral phonon radiance and the angular phonon intensity. We use material properties derived from ab initio density functional theory simulations to resolve the spatial distributions of the macroscopic variables for the following materials: gallium nitride, aluminum nitride, and gallium arsenide. We report Kapitza resistance, temperature, and thermal conductivity for these materials in 2D, and investigate thermal conductivity distributions in bulk AlN with GaN dopants of varying concentrations and physical configurations in 3D.



Using the MOOSE Framework to Model Thermoelectric Generators

Lise Charlot (Idaho National Laboratory, INL), Donna Guillen (INL)

Thermoelectric Generators (TEGs) are passive, solid-state devices that convert thermal energy into electrical energy through the Seebeck effect. These devices offer a promising solution for waste heat recovery in various applications. However, because their efficiency is relatively low compared to other power generation mechanisms, they must be meticulously designed to ensure practical usability. The performance of these devices can be modeled by solving the heat conduction and electric conduction equations with additional terms to account for the Peltier, Thomson, and Seebeck effects. The MOOSE framework provides a straightforward way to implement these effects by adding the relevant kernels to each equation. The resulting application can be used to optimize the performance of these devices while accounting for the complex properties of the material used in each leg. The implementation of the thermoelectric effects is verified through a code-to-code comparison with a commercial tool. The verification cases include a single leg with temperature-dependent material properties operating as a cooler or as a generator, for both steady-state and transient operation, and a module operating as a cooler coupled with thermal stresses. Finally, a demonstration on a module with complex leg geometry is presented to illustrate the versatility of the application.

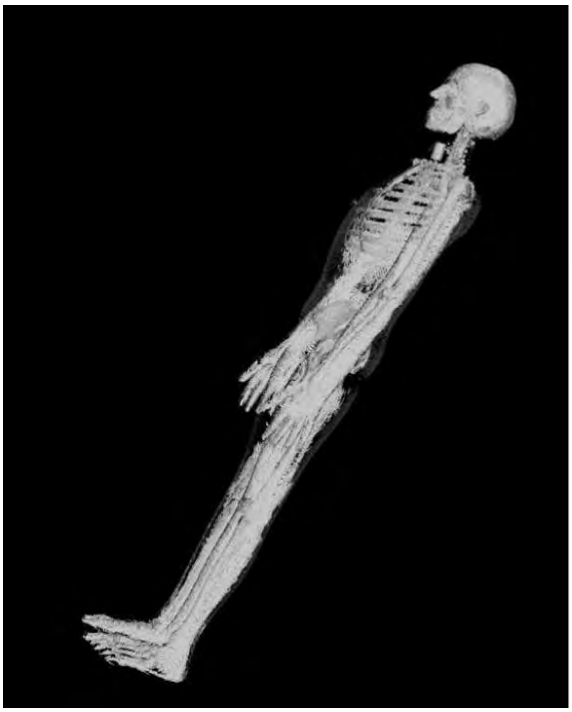


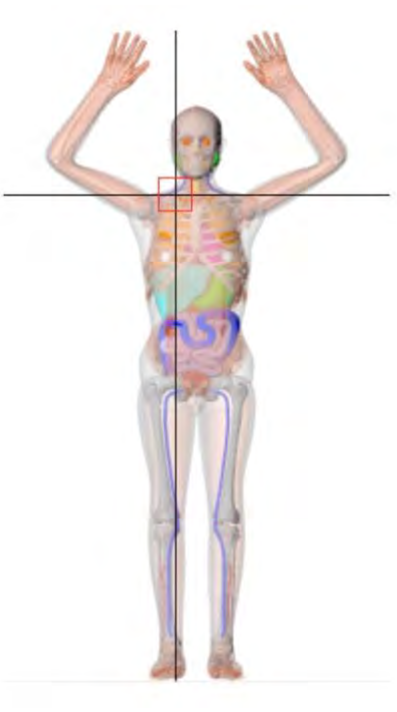
Computational Phantoms in MOOSE for Medical Physics

Matthew Anderson (Idaho National Laboratory)

The National Cancer Institute (NCI) provides a library of computational human phantoms for research purposes covering a wide range of body size-dependent children and adults for dosage calculation as part of nuclear medicine procedures. These phantoms are voxel based and are designed for use with MCNP or Geant4 but are not currently suitable for use with the MOOSE

framework. This work presents a mesh representation of the NCI reference phantoms that interoperates with the MOOSE framework to enable nuclear medicine analysis and dosimetry. We explore boron capture therapy in the context of thermal energy ranges consistent with the accelerator-based sources used for glioblastoma multiforme treatment using the phantoms. Enabling phantom capabilities with the MOOSE framework opens simulation capabilities to a wide range of nuclear medicine analyses that can complement the existing Monte Carlo approaches used in clinical treatment plans.





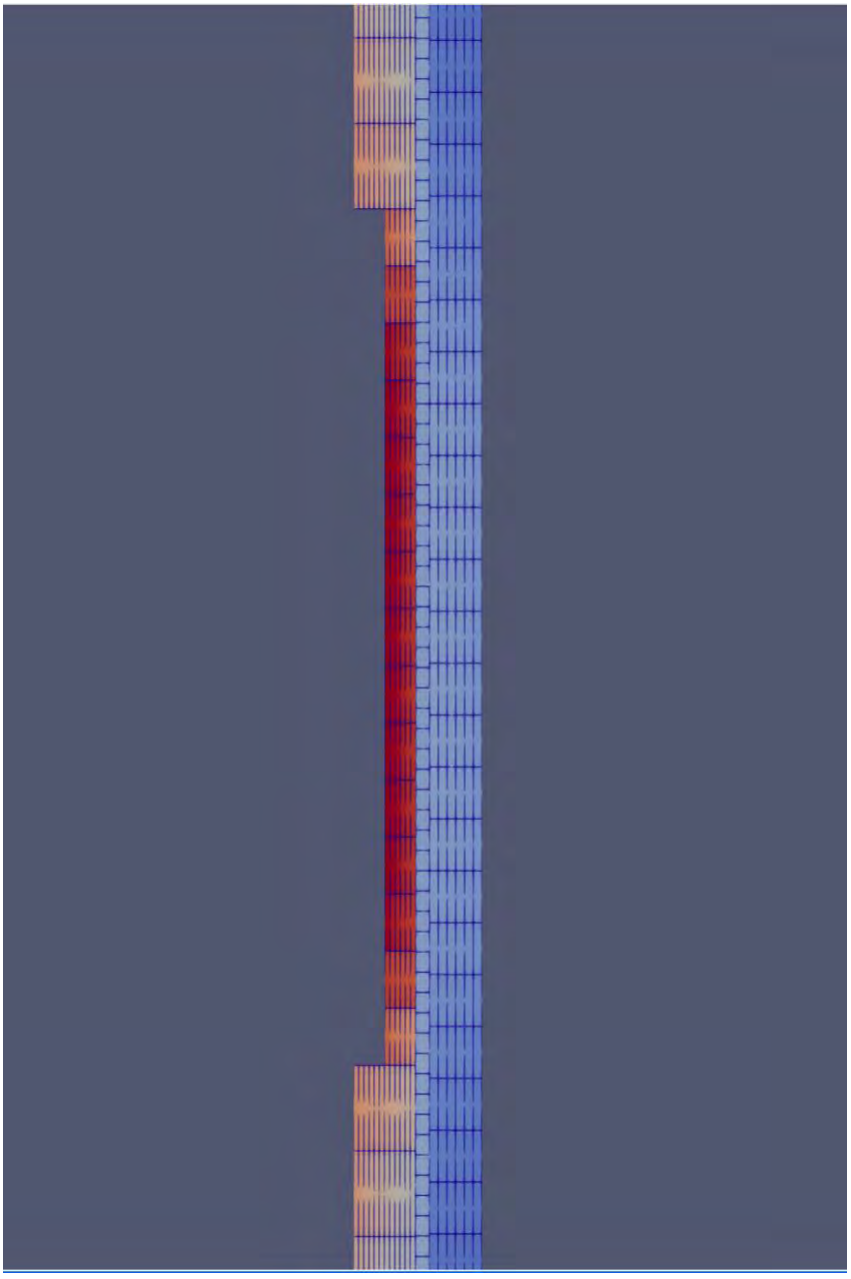
POSTER SESSION

If the poster topic was also presented orally in a session, the abstract will be listed under that session.

BISON Modeling of ZIRLO Cladding for Reactivity Initiated Accident Separate Effects
Landry Wells (University of Tennessee Knoxville)

The United States relies on light water reactors (LWRs) for its nuclear power fleet. In the wake of the beyond-design-basis accident at Fukushima Daiichi Nuclear Power Station in 2011, the department of energy (DOE) created the accident tolerant fuel (ATF) program to develop and assess potential fuel and cladding options for LWRs. For the study of these material's characteristics, both experimental and computational models are made. Oak Ridge National Laboratory (ORNL) uses modified burst tests (MBTs) for separate-effects mechanical tests in the hopes to qualify ATF cladding materials for reactivity-initiated accident (RIA)-like conditions. MBT subjects the cladding sample to the effects of pellet-cladding mechanical interaction (PCMI) that may occur during the low-temperature phase of a RIA. During the MBT, in-situ hoop strain

measurements are taken and can be used to validate BISON models of the experiment. BISON is a multiphysics fuel-performance code developed and maintained by Idaho National Laboratory (INL). By creating a mesh of the test and using known conditions, BISON can simulate the experiment and provide valuable mechanical information throughout the experiment. Future use of computer models like BISON will save the nuclear community time and costs on experiments if they can accurately predict mechanical behavior in accident scenarios. The ATF program focuses on new candidates as well as industry materials such as low oxidation zirconium by Westinghouse (ZIRLO). ZIRLO has proven reactor operation time and is still being improved. The Nuclear Regulatory Commission (NRC) believes these materials are important for the continued use of the United States nuclear fleet. This work looks to continue to validate these MBTs for ZIRLO cladding and compare the results from experimental and computational models.



Generating a High-Quality Mesh for Helicoidal Cruciform Accident Tolerant Fuel in MOOSE

Guillaume Giudicelli (Idaho National Laboratory)

Accident tolerant fuels are being investigated since the Fukushima-Daiichi accident as a technical solution to limit consequences of beyond design basis accidents. These fuels present increased physical characteristics, such as a higher thermal conductivity or improved convective heat transfer, that let them operate further from fuel failure. In this talk we will present meshing efforts for high fidelity studies of the helicoidal cruciform fuel developed by Lightbridge. Its unique shape is not currently covered by the capabilities of the Reactor module in MOOSE. In this talk, we will describe the meshing process, ensuring symmetry, volume conservation, and low skewness.

The Strength Reduction Method Applied to The Hardening Multi-Plasticity Model to Numerically Study Flank Collapses of Volcanoes

Jens Niclaes (UCLouvain)

Volcanic flank collapses are catastrophic events capable of causing significant destruction and triggering secondary hazards such as tsunamis. Strength reduction is a widespread numerical method assessing the stability of a geological edifice by gradually reducing its strength parameters. The reduction factor provoking the instability is called the safety factor. Large flank collapses occur cyclically throughout the life of a volcano. One potential cause is hydrothermal alteration, where reactive fluids and heat interact with the host rocks, altering their mechanical properties. In most volcanoes, this process negatively impacts the brittle-ductile transition of volcanic rocks, leading to a more ductile failure behavior, mainly driven by compression, instead of a brittle one, led by shear. The mechanisms behind large volcanic flank collapses remain unclear, particularly when hydrothermal alteration is involved. The impact of the ductile-brittle transition on mechanical behavior is rarely considered in flank stability assessments. Moreover, the compressive plastic cap behavior, notably present in altered volcanic rocks, is seldom modeled, even more so as the strength reduction method is followed. We conducted Finite Element Method simulations on 2D and 3D models of the Tutupaca volcano, representing its pre-collapse state in the late 18th century, under both dry and wet conditions. Using the strength reduction method, we evaluated the stability of each configuration by calculating the factor of safety and identifying the most critical failure mechanisms. The collapse was best replicated when volcanic rocks were modeled using a Mohr-Coulomb material with an additional compressive cam-clay cap, consistent with the low brittle-ductile transition seen in experimental studies on altered volcanic rocks. Including the compressive cap improved the model's predictive accuracy for collapse triggered by earthquake-induced ground acceleration. Our findings demonstrate that hydrothermal alteration impacts volcanic stability by modifying the brittle-ductile transition of volcanic rocks. This study offers key insights into the role of hydrothermal processes in volcanic flank instabilities and highlights the importance of accounting for variations in the brittle-ductile transition in stability assessments. Incorporating these variations could significantly improve future models for predicting volcanic hazards.

Developing a Coupling Between the AEGIS Charged Particle Tracking Code and MOOSE to Enable Scalable Thermal Analysis of Plasma Facing Components

Waqar Butt (UK Atomic Energy Authority)

AEGIS [1] is a new charged particle tracking code for determining steady state heat flux distributions on complex engineered CAD surfaces due to charged particles in Tokamak reactors. As particles move around inside a reactor, some of them will slowly drift towards the edge of the plasma and cross over the last closed magnetic flux surface and escape confinement - they are then carried along magnetic field lines and strike Plasma Facing Components (PFCs). AEGIS operates by mapping heat flux from particles which cross that boundary onto faceted meshes of these PFCs. It uses a relatively simple model of particle motion (axi-symmetric equilibria along with a particle guiding center approximation) but can map heat flux onto high-fidelity models of complex CAD surfaces. The Direct Accelerated Geometry Monte Carlo (DAGMC) toolkit is used to provide a solution for storing the mesh and perform raytracing against that mesh to precisely determine where on the faceted CAD the particle strikes. In this work we present a proof of concept of a coupling between AEGIS and the MOOSE framework, that can be used to perform a thermal analysis on PFCs due to the heat flux arising from charged particles. AEGIS has been developed with the intention of replacing an existing serial code (SMARDDA-PFC) for charge particle tracking and has a similar workflow with Ansys. AEGIS has also recently been extended with parallel algorithm implementations via MPI with reasonable strong and weak scaling, over the parallelised portions of the code, out to at least 1000 cores. Thus, we demonstrate how this new AEGIS-MOOSE coupling is capable of replacing an existing engineering workflow with a new scalable workflow that relies on MOOSE. The Coreform Cubit meshing software has been used to produce both faceted meshes for DAGMC and FEM meshes for MOOSE with the same CAD files. This work aims to develop a tighter integration between AEGIS and thermal simulations in MOOSE, building on previous demonstration workflows with file-based coupling between tools. [1] W. K. Butt *https://github.com/aurora-multiphysics/aegis*. This work has been funded by the Fusion Futures Programme. As announced by the UK Government in October 2023, Fusion Futures aims to provide holistic support for the development of the fusion sector. The author would also like to thank D. Brennand, N. Carey and A. Khan for their contributions and discussions in previous demonstrative workflows.

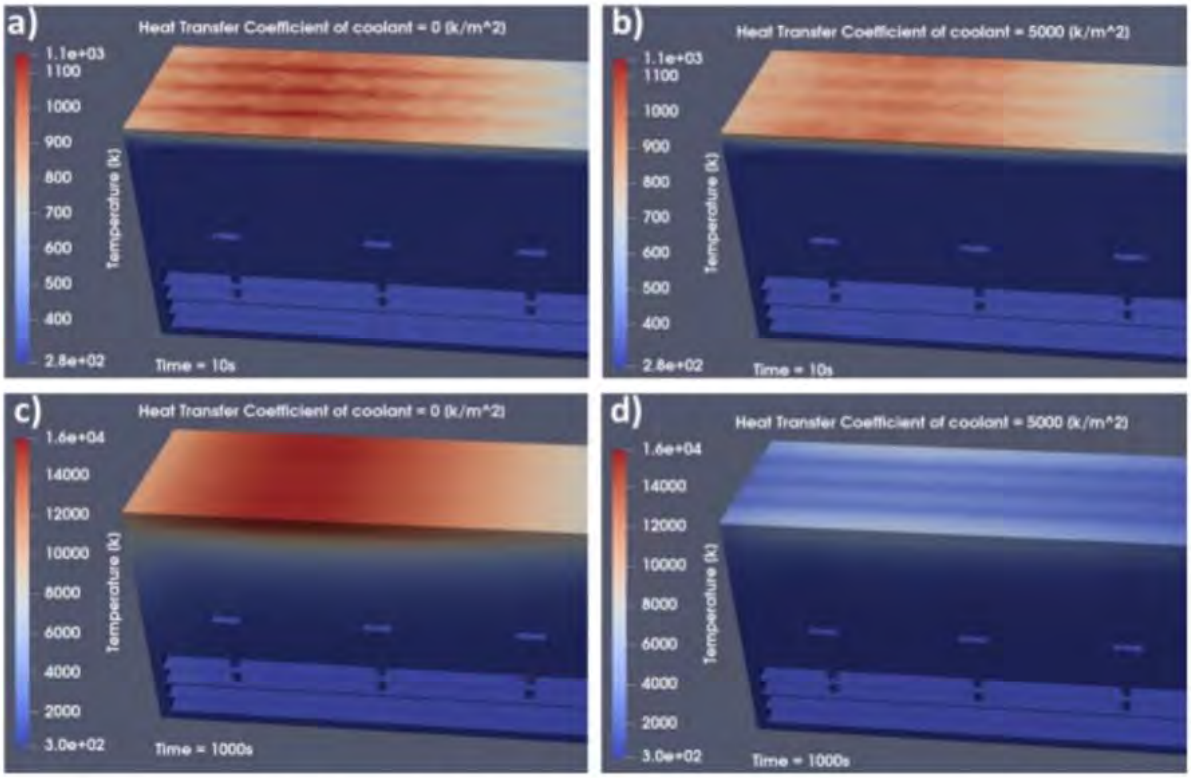


Figure 1: Thermal conduction solved for temperature in MOOSE with heat flux produced by AEGIS. a) Early timestep with no cooling. b) Early timestep with cooling. c) Late timestep with no cooling. d) Late timestep with cooling

Using MOOSE to Quantify the Impact of Solid Precipitates on Bubble Coalescence

Tanvir Sakib (University of Florida)

Uranium dioxide (UO2) is one of the most used light water reactor fuels due to its chemical stability and high melting point. During reactor operations, gaseous fission products (Xenon and Krypton) are generated and form fission gas bubbles, which impact the fuel performance. Moreover, solid, insoluble metallic and oxide fission products precipitate, which could also affect fuel efficiency. The impact of solid fission products and their interaction with fission gas bubbles was not studied extensively to date. In this work, we employ the Multiphysics Object Oriented Simulation Environment (MOOSE) phase-field module to investigate interactions between solid fission products and fission gas bubbles. We explore the impact of static precipitates on intergranular bubble coalescence. We find that the fission gas bubbles that interact with solid fission products coalesce slower compared to the case without solid fission products. Furthermore, we study how solid fission product dimensions can affect bubble separation; we show that bubbles can readily separate from smaller precipitates while it is harder to separate from larger ones. Additionally, the position of the solid fission products with respect to the bubbles plays an essential role in bubble separation. Finally, we find that, in some cases, bubbles completely fail to escape the precipitates due to their respective arrangements.

Digital Rock Physics Framework for Energy Geomechanics

Sijmen Zwarts (TU Delft)

Digital Rock Physics (DRP) is a framework which uses high resolution micro-CT scans of real rock samples to create digital models. These models enable Finite Element simulations of the microstructural physical behavior of the rock samples, replacing the need for destructive laboratory experiments. The physical behavior on the microscale is upscaled to a larger scale to have more predictive power in our macroscopic models. This poster presents the DRP framework of and presents several advancements om multiple aspects of the DRP, including identifying the Representative Elementary Volume (REV), simulating coupled multi-physics processes, and improving upscaling techniques. These developments contribute to a more accurate characterization of rock properties, supporting applications such as reservoir modeling and subsurface storage.

Tuesday, March 11

PLENARIES

How We Learned to Stop Worrying and Love MOOSE

Andy Davis, United Kingdom Atomic Energy Authority

In this talk I will cover our MOOSE journey at the United Kingdom Atomic Energy Authority; the circumstances that lead to be it being introduced, the barriers and challenges we faced, and the things that we produced. I will cover our broader aspirations for simulation in our part of the fusion arena, and how it fits into the broader simulation roadmap at UKAEA.

Tales From the Depths

Andy Wilkins (Commonwealth Scientific Industrial Research Organization, CSIRO), Chris Green (CSIRO), Thomas Poulet (CSIRO), Heather Sheldon (CSIRO)

The Earth's subsurface has long fascinated us, holding both mysteries and treasures. My presentation will take you on a journey through the subsurface, using MOOSE to quantify and explore its mysteries. We will delve into topics such as groundwater modelling, multiphase flows, rock dynamics, and heat. I shall highlight CSIRO's work with MOOSE, which supports emissions reduction, resource extraction and environmental management.

Recent Advances in Regularized Models of Fracture and Accompanying Discretization Methods

John Dolbow, Duke University

We provide an overview of several recent advances in models for the fracture mechanics of elastic brittle materials. These advances are changing the focus in the community from models and simulations of crack propagation to those for crack nucleation. At this point it is clear that at least

three intrinsic macroscopic material properties govern fracture nucleation in elastic brittle materials: i) the elasticity; ii) the strength; and iii) the fracture toughness or critical energy release rate. Of these, material strength has been the most misunderstood and overlooked, despite its central role in governing crack nucleation under a broad set of conditions. Precisely how cracks nucleate and transition to propagation, and how descriptions of strength should be interlaced with Griffith-like energetics in models for fracture has been a subject of study for decades. We will focus attention on an emerging class of regularized models of the phase-field type that are complete in the sense that they allow for the representation of an arbitrary strength surface. This completeness is what has permitted these models to move beyond mere calibration against particular experimental observations. Select examples from quasi-static and dynamic fracture that illustrate the interplay between strength and energetics will be shown. The challenges and opportunities this new perspective provides for research in numerical methods will be discussed, as well as an outlook into modeling fracture nucleation beyond the basic setting of elastic brittle materials.

AI/ML panel

Yang Liu (Texas A&M University), Daniel Schwen (Idaho National Laboratory, INL), Mengnan Li (INL), Som Dhulipala (INL), Gary Hu (Argonne National Laboratory)

This session will delve into the transformative potential of scientific machine learning (SciML) to advance computational simulations across various energy solutions, including nuclear fission, geothermal, and nuclear fusion. Key discussion points will include the integration of Large Language Models (LLMs) to improve user experience through a lightweight, open-source LLM agent that assists with keyword searches, documentation retrieval, and input file guidance. The panel will explore the development of a pipeline for a vector database of MOOSE documentation and input files, preparing MOOSE for versatile LLM integration and research. The session will also cover the implementation of surrogate models using torch models such as feed-forward neural networks, with a focus on GPU evaluation and integration into a NEML2-based constitutive model. Attendees will gain insights into the combination of inner-loop modeling with physics-based ML, and the integration of operator learning within MOOSE to provide excellent initial guesses for inner-loop solves, thereby accelerating convergence. A significant topic of discussion will be the generalization of inner-loop ML/operator learning models across multiple physics of interest to the MOOSE community, ensuring their trustworthiness, and hybrid physics-based and data-driven approaches to scientific discovery. The panel will address outer-loop approaches for optimization, uncertainty quantification, inverse problems, data assimilation, and control, alongside the use of active learning with the MOOSE stochastic tools module for intelligent data acquisition from large simulations or experiments. Challenges related to coupled physics across multiple scales during active learning and the propagation of uncertainty sources across scales will also be discussed.

NUCLEAR 3

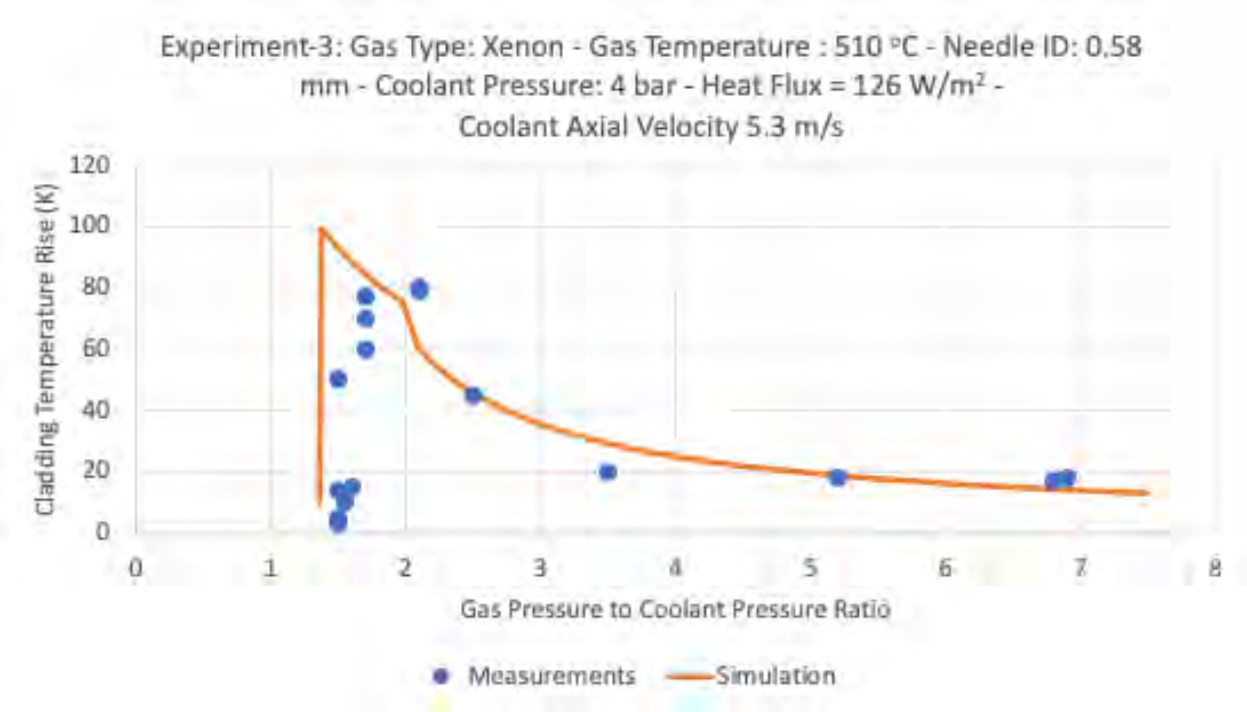
Modeling Clad Damage Propagation in Liquid Metal Fast Reactors Using MOOSE-SC

Aydin Karahan (Argonne National Laboratory)

Quantifying fuel failures is a critical task for licensing an advanced reactor concept. Uncertainties tend to increase with irradiation-induced changes, fuel/cladding interactions, and corrosion. Failures typically occur in exceptional pins subjected to adverse conditions. Modeling the probabilistic nature of cladding failures and post-failure degradation is crucial for understanding fuel failures and accident progression. Cladding failure in adversely affected pins, followed by their dispersal, can degrade heat transfer in neighboring fuel pins and reduce coolant flow rate. This degradation can lead to operational conditions requiring evaluation of successive thermal creep rupture risks especially in limiting transient scenarios at elevated temperatures. The Clad Damage Propagation (CDAP) model was developed and implemented into MOOSE-SC subchannel analysis tool to address these phenomena. It includes:

1. Probabilistic Failure Simulation: Quantifying fast reactor fuel failures based on a failure probability density function for each pin.
2. Post-Failure Dynamics: Modeling depressurization, fission gas dispersal, and its impact on neighboring pins, including heat transfer degradation.
3. Two-Phase Flow Behavior: Predicting interactions between fission gas and liquid metal in the coolant channel, including void fraction impacts on pressure drop, mass flow rate, and heat transfer.
4. A one-dimensional, time-dependent finite volume fuel pin temperature distribution model.

CDAP incorporates a simplified set of constitutive relations for metal fuel performance, including plenum pressure, cladding stress, eutectic formation, and creep rupture. The model also includes a submerged fission gas jet submodel to predict jet velocity, diameter, and entrained liquid coolant volume fraction as a function of downstream distance. This submodel is coupled to a heat transfer model for the impingement region of the target neighbor pin. A gas mass tracker with void fraction calculations identifies axial nodes with two-phase flow conditions, linking these to further reductions in creep rupture margins during post-failure depressurization events. The CDAP model has been validated against submerged gas impingement experiments using electrically heated pins, demonstrating promising results for reactor safety analysis and licensing of advanced reactor concepts.

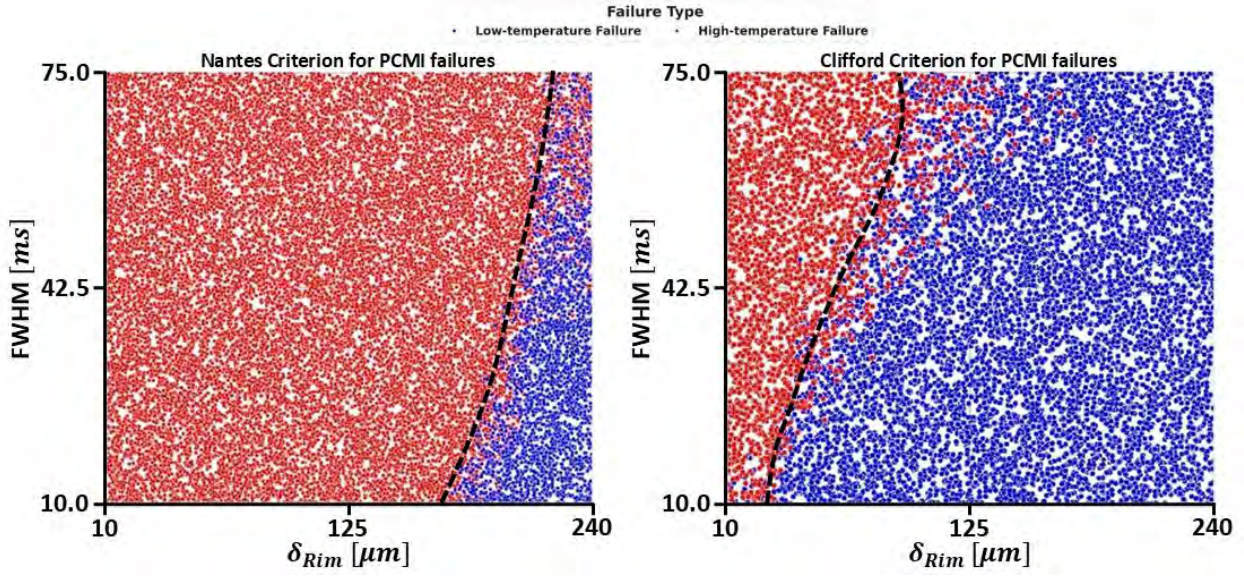


Toward Development of a Low-Temperature Failure Envelope of Cases for High-Burnup RIAs Under PWR Operational Conditions

Luiz Aldeia Machado (The Pennsylvania State University, Penn), Katheren Nantes (Penn), Elia Merzari (Penn), Lise Charlot (Idaho National Laboratory), Arthur Motta (Penn)

A Reactivity-Initiated Accident (RIA) is a design-basis accident that occurs when the reactor loses one of its control rods. A reactivity insertion will follow such events, drastically increasing the fuel pellet's temperature and volume due to thermal expansion. The fuel pellet and the cladding will interact mechanically, which could lead to cladding failure. This work presents the development of an envelope of cases where low-temperature failures are more likely to happen for high-burnup fuels under PWR operational conditions. A coupled computational model between the nuclear fuel performance code BISON, MOOSE's Thermal-Hydraulic Module (MOOSE-THM), and MOOSE's Stochastic Tools Modules (MOOSE-STM) was created to study the thermal-hydraulic behavior of a high-burnup fuel rodlet during the first stages of an RIA transient, allowing us to identify three scenarios: the system reached CHF, leading to high-temperature failure, the system failed due to PCMI, or the system survived the whole transient without failing. To address these three scenarios, a total of 100,000 model replicates varying the power pulse total energy deposition, power pulse width, hydride rim thickness, pitch-to-diameter ratio, coolant mass flux, and coolant inlet temperature were performed through the MOOSE-STM using a PCMI correlation that accounts for the local hydride concentration to determine if the system failed or not. We validate our computational results against the available CABRI REP-Na3 test data and also against BISON standalone simulations. Our results suggest that the hydride rim thickness will play a major role in determining the system's failure type, with the RIA power pulse width having the second most relevant impact on the failure type. By isolating the parameters that have the most significant

impact on the type of failure our system undergoes during an RIA, we were able to determine an analytical expression for the boundary that separates the regions where PCMI or CHF are more likely to happen as a function of the hydride rim thickness and the power pulse width.

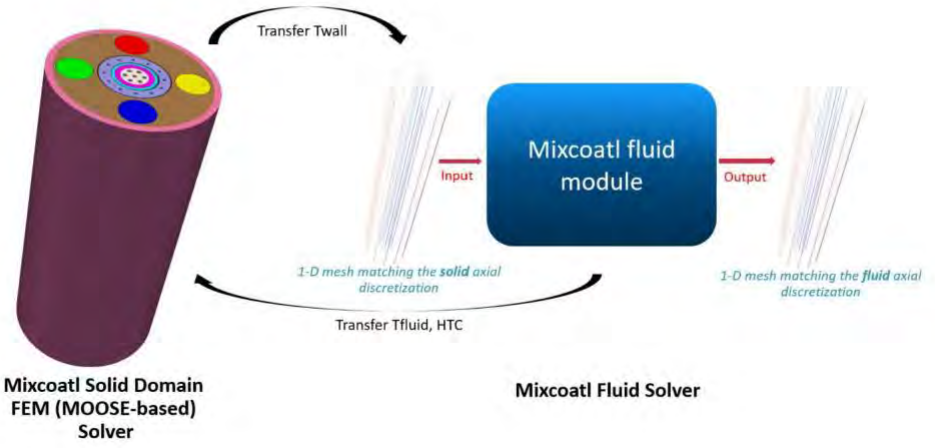


MixcoatlTM 2.0: BWXT's Improved MOOSE-based Conjugate Heat Transfer Software for Reactor Applications

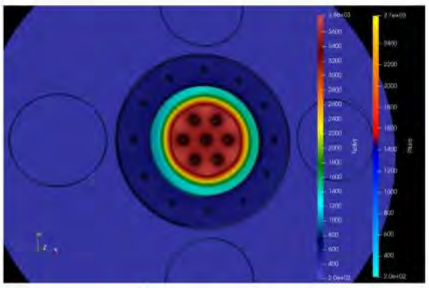
Vincent Laboure (BWXT), Phil Hegedus (BWXT), Nathaniel Peat (BWXT), Bryan Zilka (BWXT), David Leazer (BWXT), Ryan Kitchen (BWXT), Rebecca Owston (BWXT)

Mixcoatl [1,2] is a MOOSE-based conjugate heat transfer software designed for the analysis of space and terrestrial nuclear reactors. Its growing user base and the variety of projects within BWX Technologies relying on its capabilities has amplified the need for increased code performance. MixcoatlTM 2.0 was deeply restructured to leverage the MOOSE framework more efficiently, specifically to enhance the coupling between the solid and fluid equations. On a large space nuclear model (~6M elements and ~1000 cooling channels), the code is now 3x faster, with a memory usage decreased by 16% and an input file 23x shorter, for virtually identical results. In addition, this new code structure opens the door for more advanced multiphysics transient capabilities â€“ by leveraging MOOSE's native ability to (1) use different time steps for the solid and fluid solves and (2) couple to other MOOSE-based applications (Griffin, BISON, etc.).

1. Pivovar, R., & Owston, R. (2023). Mixcoatl Software (Part 1): Coupled Thermal Physics and Mechanics for Efficient Engineering Design. Nuclear Science and Engineering, 197(4), 676-685. https://doi.org/10.1080/00295639.2022.2154114
2. Pivovar, R., & Owston, R. (2022). Mixcoatl Software (Part 2): Verification of 1D Fluid Flow Methods Coupled to 3D FEM Thermal Diffusion Models. Nuclear Science and Engineering, 197(4), 686-702. *https://doi.org/10.1080/00295639.2022.2126718*



- Mixcoatl was rewritten to more efficiently leverage the MOOSE framework for solid-fluid coupling
- Runtime, memory usage and input file automation were all improved with Mixcoatl 2.0.



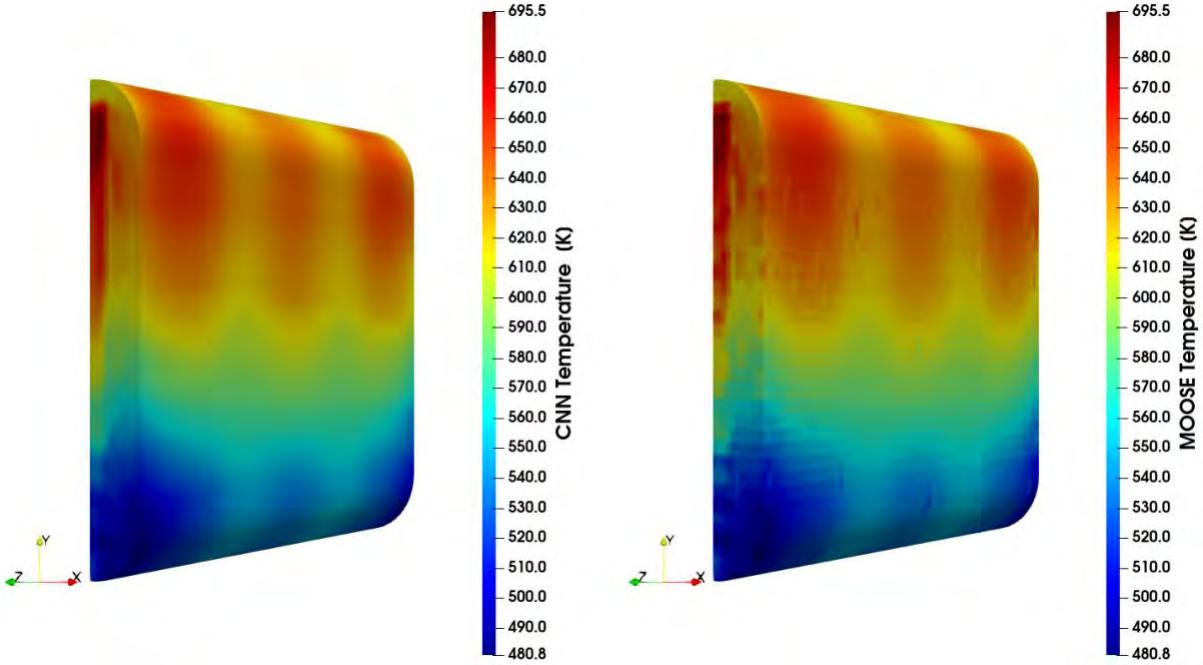
Large NTP model	Execution Time	Max Memory Usage	Input File Length
Legacy Mixcoatl	20874 s	12360 MB	48691 lines
Mixcoatl 2.0	7172 s	10387 MB	2153 lines
Improvement	2.91x	1.19x	22.6x

Temperature Field Reconstruction of Surfaces Heated Through Radiative Heat Transfer Using Convolutional Neural Networks

Luiz Aldeia Machado (The Pennsylvania State University, Penn), Victor Coppo Leite (Penn), Elia Merzari (Penn), Lesley Wright(Texas A&M University, TAMU), Pramatha Bhat (TAMU), Yassin Hassan (TAMU), Roberto Ponciroli (Argonne National Laboratory, ANL), Lander Ibarra (ANL)

Diverse applications require us to know the value of a given physical quantity in real-time. For many applications, we can rely on probes to fulfill this task. However, this approach can be challenging when we need to know these quantities in many locations over a given domain due to the spatial limitation involved. In this context, using Convolutional Neural Networks (CNN) can offer a good

option to deal with such a problem. A well-trained physics-informed CNN can reconstruct the distribution of a given physical quantity over a domain using only a few sensors, allowing us to reconstruct the desired field distribution even in a limited space or complex geometries where a large array of sensors remains impractical. This work will present the initial approach to developing a real-time tool for monitoring the thermal behavior of nuclear reactor pressure vessels. Based on an experimental setup, the team developed a computational model using the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework, where the Ray Tracing and Heat conduction modules were used to evaluate the temperature distribution over a convex metal surface heated through radiative heat transfer. This metal surface represents a section of a heated nuclear reactor vessel wall. We verified our computational model against the available experimental data. Part of the data generated by the MOOSE model was used to train the Convolutional Neural Network to reconstruct the vessel wall's outer surface temperature. The CNN generalization was then verified against the experimental and computational data. The predicted temperature distribution over the vessel's outer wall presented an R-square metric of 0.9991 when compared against the MOOSE model.



FUSION 1

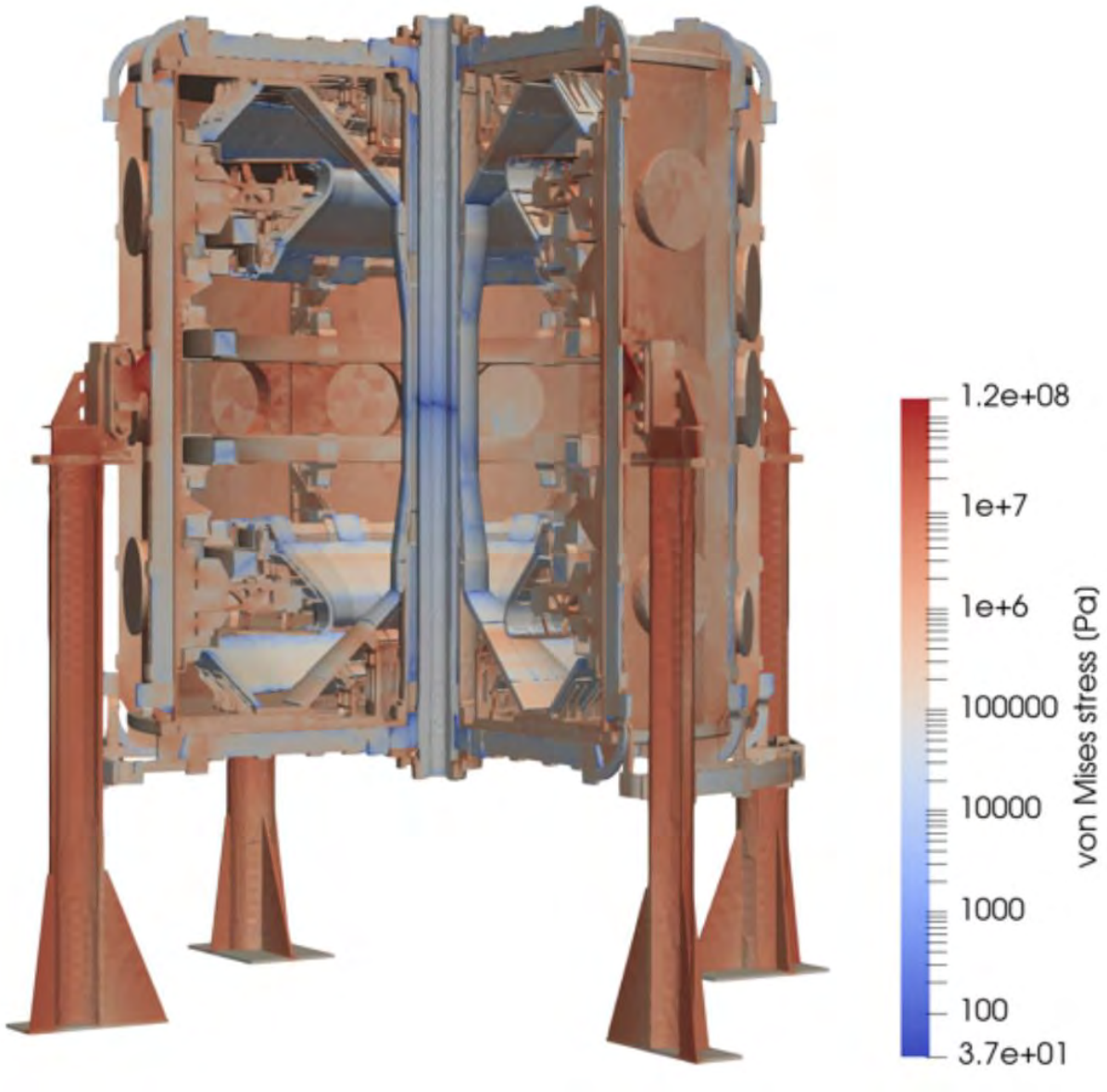
Stress, Strain, Neutron Transport and Radiation Effects in a Full Fusion Tokamak Device: A Virtual MAST-U Study

Luca Reali, William M.E. Ellis, Ander K. Gray, Max Boleininger, Helen M. Brooks, James Buchanan, Andrew Davis, and Sergei L. Dudarev (UK Atomic Energy Authority)

A virtual model for a tokamak fusion reactor involves linking the concepts and algorithms that span atomistic to macroscopic length scales and necessarily include the treatment of many domains of physics and engineering [1, 2]. An in-silico model for the tokamak prior to its construction is

expected to enable many critically significant technological developments and applications, to decrease the overall development time and to decrease the costs for this development. First, it should enable screening competing reactor concepts on a scale and at pace not attainable using a design-by-experiment approach. Second, it should allow the consideration of radiation damage at neutron energies and component sizes that are not yet accessible to experiment [3,4], and the treatment of closely related phenomena, for example the enhanced tritium retention in the reactor materials exposed to radiation [5,6]. In all these cases, formulating and implementing the linked models require considerable care and thoroughness as poorly controlled simplifications and uncertainties can have a large effect on predictions. Here, we develop a finite element model for the entire MAST-U spherical tokamak, presently operating at UKAEA. The model involves 127 million finite elements and is parallelised over hundreds of processors using the MOOSE software. Structural calculations have been performed under purely mechanical loads such as gravity or a dynamical earthquake-like excitation. The model can also be coupled to neutron transport Monte Carlo simulations, on the same full-device scale and the same mesh using parallel neutron transport code OpenMC [7]. To represent radiation damage effects in the form of spatially varying swelling, we parametrise a surrogate model using a massively parallel software for atomistic simulations, the molecular dynamics package LAMMPS. We explore how to transfer information from the domain of neutronics to the domain of structural calculations through the detailed analysis of fundamental radiation effects in materials. Preliminary results from this work were published in [8].

1. T. R. Barrett, et al. IEEE Transactions on Plasma Science 47, 889 (2018).
2. B. W. Spencer, et al, Nuclear Technology 207, 981 (2021).
3. S. L. Dudarev, et al, Nuclear Fusion 58, 126002 (2018).
4. L. Reali, et al, Nuclear Fusion 62, 016002 (2022).
5. D. R. Mason, et al, Phys. Rev. Materials 5, 095403 (2021)
6. J. Dark, et al, Nucl. Fusion 64, 086026 (2024)
7. Paul K. Romano, et al, Ann. Nucl. Energy, 82, 90â€“97 (2015)
8. Reali, Luca, et al. EPJ Web of Conferences. Vol. 302. EDP Sciences, 2024.

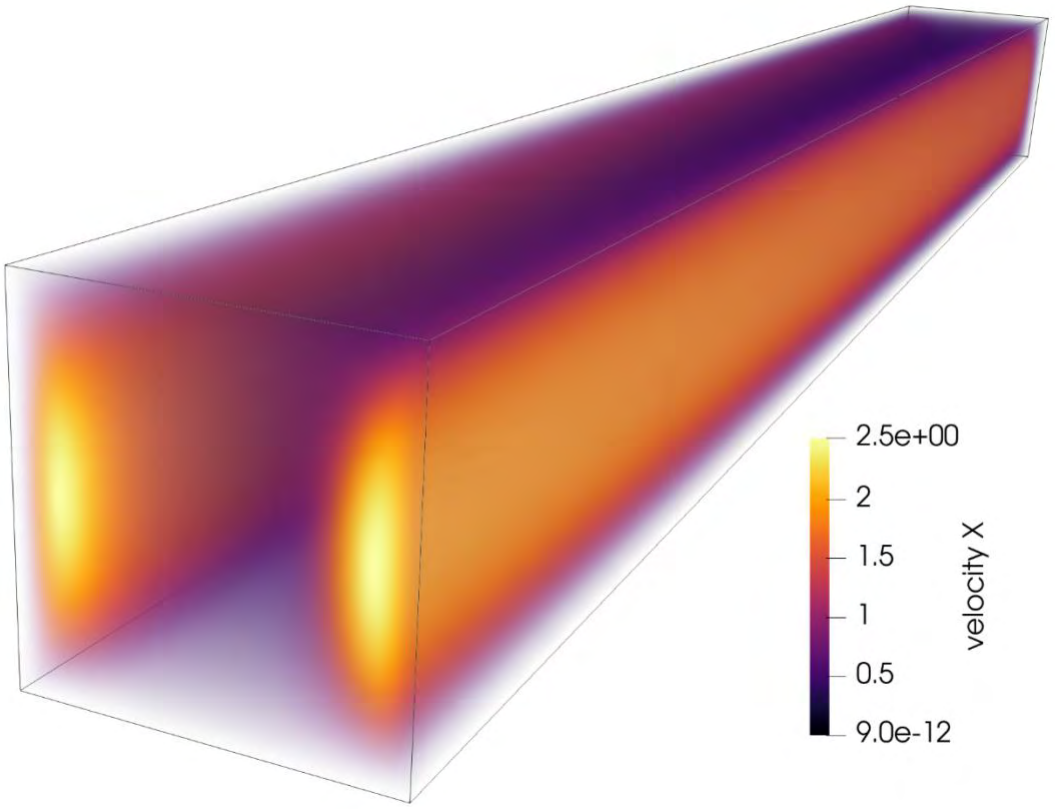


Development of Liquid-Metal MHD Simulation for Fusion Multiphysics in MOOSE

Rupert W Eardley-Brunt (UK Atomic Energy Authority, UKAEA), Daniel R Ward (Hartree Centre, STFC), Gerasimos Politis (UKAEA), Pranav Puthan (UKAEA), Aleksander J Dubas (UKAEA), Andrew Davis (UKAEA)

An essential aspect of developing fusion technology, supporting current experiments, and leading to a commercially viable power source, will be the ability to perform accurate, predictive simulation of fusion components. Breeding blankets are one of the challenging components which must be studied, and some blanket designs include the flow of liquid metals which are dominated by magnetohydrodynamic (MHD) effects due to the strong interaction between the conducting fluid and the magnetic fields confining the plasma. Developing and validating accurate numerical solvers for these systems has been a topic of much interest in recent years. Bringing such solvers

into the MOOSE ecosystem, enabling coupling to the physics already implemented in MOOSE, is a key step towards accurate multiphysics simulation of liquid-metal breeder blankets. This work presents ongoing efforts to implement liquid-metal MHD solvers into MOOSE, involving a variety of approaches from directly implementing the equations in MOOSE to coupling external solvers. The tight coupling involved, even with the simplifications of the inductionless approximation, leads to a system of equations which is challenging to solve, with efficient solution of these systems standing out as an essential step in enabling simulations of full blankets. Liquid-metal MHD simulation coupled to the complex physics involved in breeding blankets, including thermal, structural, and electromagnetic coupling to the surrounding domains as well as neutronics and tritium breeding, enabled by the multiphysics coupling framework in MOOSE, will be an invaluable tool in the development of fusion technology.

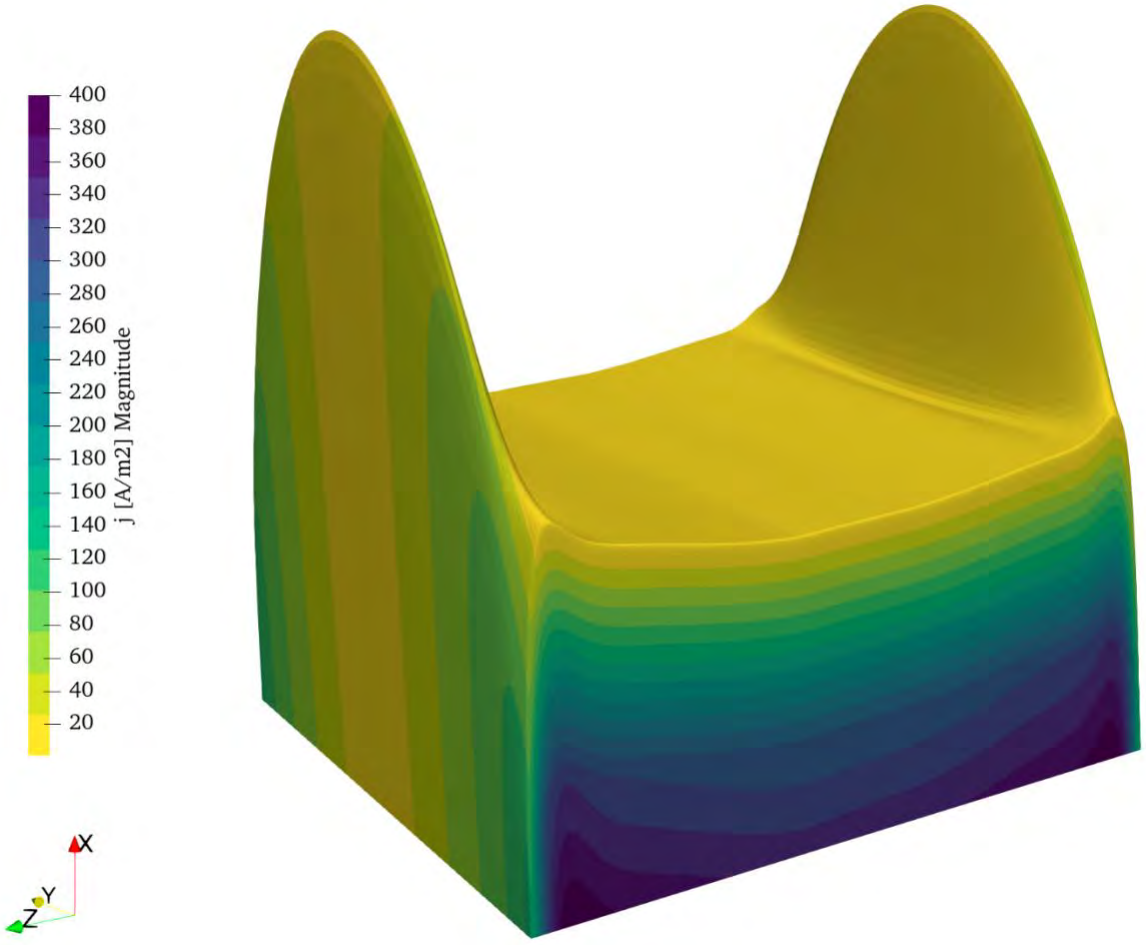


Development of a Simulation Tool for Liquid Metal MHD Flows in MOOSE

Daniel Suarez (Oak Ridge National Laboratory, ORNL), C. Isenhour (Idaho National Laboratory), P. Humrickhouse (ORNL)

Liquid metal (LM) flows are among the most advanced proposals for breeding blankets in future fusion reactors. In recent years, the Dual Coolant Lead Lithium (DCLL) has been thoroughly studied in the US and in Europe due to its advantages in neutron multiplication, tritium breeding ratio (TBR), shielding, and high thermal efficiency. More recently, private companies have proposed the flow of

pure liquid lithium (also a LM) in the breeding blanket channels. The flow of a LM under the influence of the strong reactor magnetic field interacts to produce the so-called magnetohydrodynamic (MHD) effect, a volumetric force that influences flow field. MHD flows in a real fusion power plant breeding blanket will feature fringing magnetic fields, strong thermal gradients, and different electrical conductivity of the channel walls. All these situations will strongly affect the velocity distribution, affecting the pressure drop experience by the flow and the transport of heat and tritium, which are crucial phenomena in any fusion power plant. In this work, we summarize advances in the development of a simulation tool in MOOSE to predict the MHD effect in liquid metal breeding blankets. We focus on explaining the physical and numerical models implemented in the code, as well as the initial verification and validation activities according to well-established international benchmark cases.



NUCLEAR EXPERIMENTAL DESIGN 1

Thermal Property Inversion with Lock-in Thermography

Lynn Munday (Idaho National Laboratory, INL), Max Nezdyur (INL), Zilong Hua (INL), Murthy Guddatti (North Carolina State University)

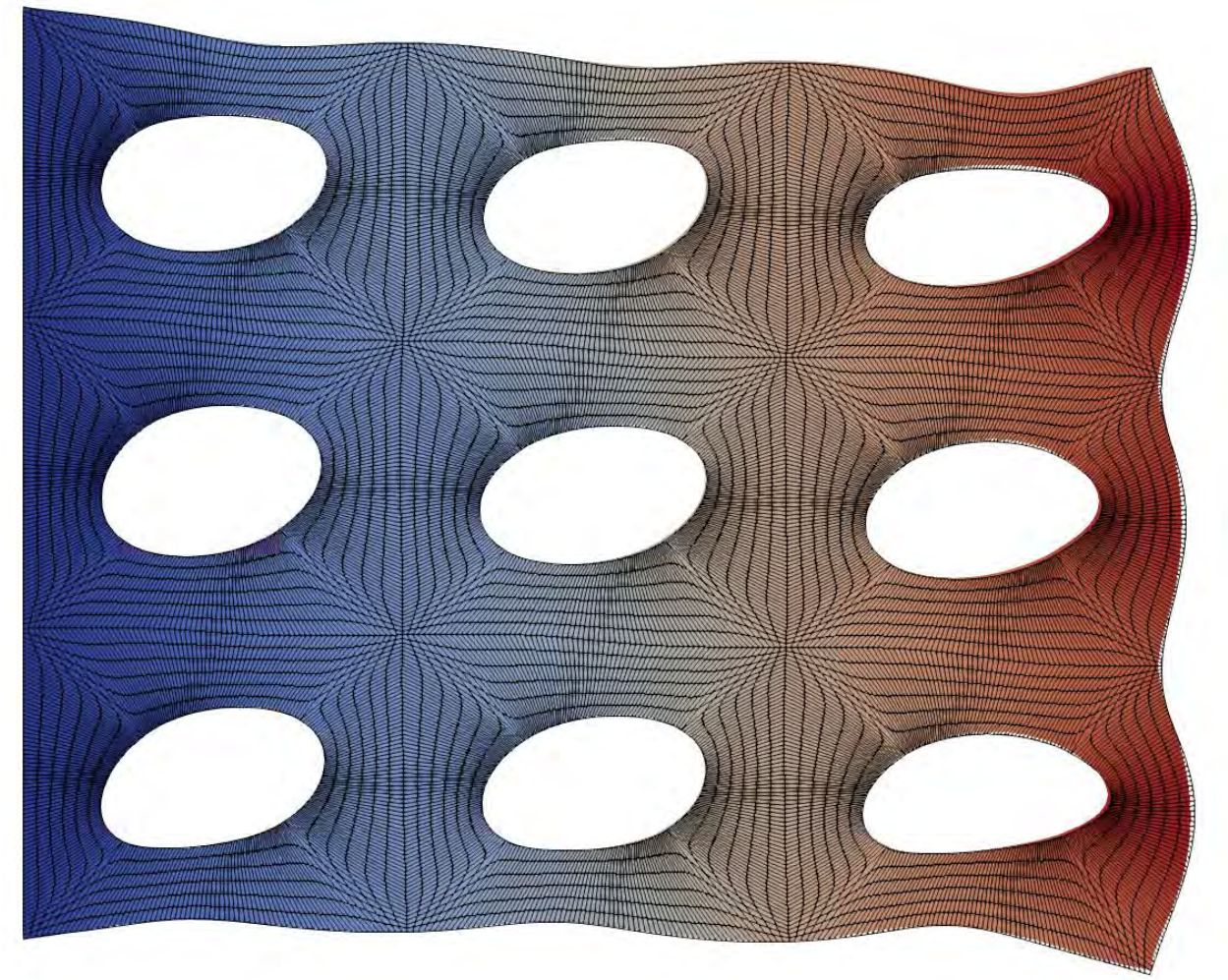
Nondestructive evaluation (NDE) capabilities at Idaho National Laboratory (INL) have been developed for characterizing parts and materials in extreme environments unique to INL's mission; among these are Lock-in Thermography (LIT). LIT excites the surface with a time-harmonic thermal source, resulting in a temporally modulated temperature field nearby. Measurements of the temperature field are used to determine the underlying material structure. In this work, the optimization module in MOOSE is used to determine a material property map from the LIT temperature field by solving an inverse problem. The forward model of the LIT process is modeled in the frequency domain. The inverse problem is solved with Multi-Resolution Full Waveform Inversion (MRFWI) where the low frequency LIT data provides a coarse material property map that is refined with higher frequency LIT data. MFRWI makes use of multiple sets of experimental data where low frequency data is used to provide a coarse estimate of the material properties at larger depths. This coarse estimate is then used as an initial condition to regularize the optimization problem at higher frequencies where more parameters are being inverted for to providing the higher resolution imaging. Multiple experiment MRFWI is applied to experimental data collected from a complex advanced manufactured component. The resulting material property maps using computational inversion are compared to those found using analytic methods which do not account for complex geometries and changing properties.

An Element Reduced Order Model Framework for Lattice Structures with Geometric Parameterization

Max Nezdyur (Idaho National Laboratory, INL), Lynn Munday (INL)

Finite element analysis of complex lattice structures often requires significant computational resources, limiting the ability to perform rapid design iterations or large-scale simulations. To address this challenge, we present a novel reduced-order modeling (ROM) approach for efficiently simulating parameterized lattice geometries in finite element analysis. Our method introduces a geometrically parameterized reduced-order model that not only significantly accelerates simulation times while maintaining high accuracy but also offers a high degree of flexibility. The ROM basis, generated using higher-order elements, ensures that the bases match at interfaces, allowing for versatile combinations of ROM elements into various lattice geometries. This adaptability enables the exploration of a wide design space with minimal computational overhead. To efficiently and accurately capture changes in the reduced system due to geometric variations, we implement matrix discrete empirical interpolation (MDEIM). This technique allows for rapid updates of the reduced system matrices, further enhancing the computational efficiency of our approach. Our method leverages the MOOSE framework, specifically utilizing its multiapp system. We structure the simulation with a main app containing super elements, complemented by sub-apps for each ROM element. This architecture enables efficient generation of the reduced system and streamlined solution computation. Our approach significantly reduces computational time

compared to traditional full-order models while maintaining a high degree of accuracy. This makes it particularly suitable for applications involving complex lattice structures in fields such as materials science, structural engineering, and additive manufacturing. The ability to rapidly evaluate multiple lattice configurations opens new possibilities for design optimization and material property tuning in these domains.



Modified Burst Testing for Reactivity Initiated Accident Separate Effects Testing on Cladding: from Experimentation to Modeling

Jennifer I. Espersen (University of Tennessee-Knoxville, UTK), Nicholas R. Brown (UTK)

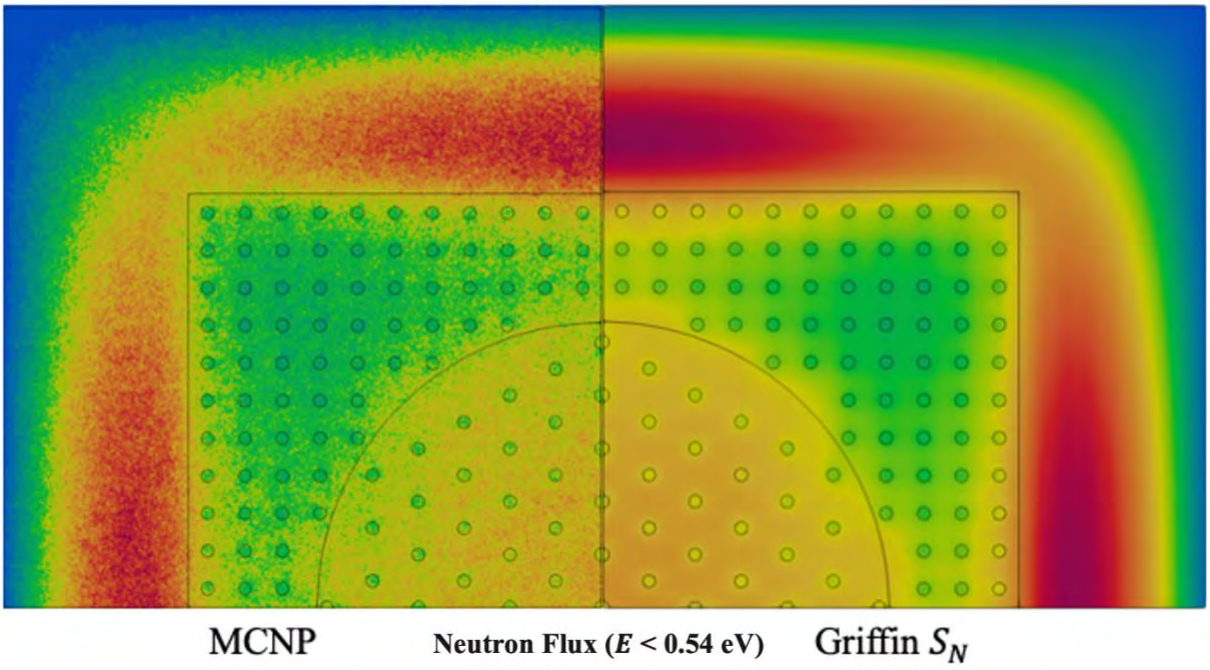
Light water reactors (LWRs) make up the fleet of commercial nuclear reactors presently producing electricity in the United States. Accident tolerant fuels (ATFs) are fuel and cladding systems for LWRs that have improved performance under transient conditions when compared with UO2 and Zircaloy, which make up current fuel systems. To qualify ATF materials for reactor operation, a combination of experiments and computational models are used. At Oak Ridge National Laboratory (ORNL), a modified burst test (MBT) has been employed to carry out separate-effects mechanical tests aimed at qualifying ATF claddings for reactivity-initiated accident (RIA)-like

conditions. MBT experimentally simulates the effects of the pellet-cladding mechanical interaction (PCMI) that may occur during the low-temperature phase of an RIA. During these tests, a high-speed camera records images of the deforming cladding specimens for analysis with digital image correlation (DIC). DIC is an analysis technique that allows for the calculation of full-field in-situ hoop strains of the cladding. These hoop strain values are used to validate BISON models of the experiment. Current efforts are to model experiments conducted on chromium-coated zircaloy-4 cladding specimens. The chromium coating provides a protective layer to the cladding that helps prevent hydride pickup and high-temperature corrosion. The MBT setup consists of a driver tube in which hydraulic oil is rapidly injected. The driver tube has a thin-walled region which expands under this pressurization, mimicking a thermally expanding fuel pellet. An adhesive is used to secure a cladding sample around the driver tube. The driver tube's expansion provides a force to the cladding that is similar to PCMI. To accurately model this experiment in BISON, a custom mesh was created to model the driver tube, adhesive, cladding, and coating. For comparison to DIC strain results, the mesh is sliced to output an average strain over the same area from which the DIC strain is calculated. In the work presented herein, the experimental conditions and results are compared with the model created in BISON.

Deimos, an Advanced Reactor Testbed and Criticality Experiment

Alexis Maldonado (Los Alamos National Laboratory)

Deimos is an advanced criticality experiment planned for 2024 at the National Criticality Experiment Research Center (NCERC). Deimos is intended to act as a testbed to host different advanced reactor designs to increase confidence in a conceptual reactor by validating nuclear data, modeling, and simulation codes. This work presents upfront modeling and simulation efforts for Deimos, such as neutronics and kinetics analyses with codes such as MCNP® and MOOSE/Griffin.



GEOSCIENCE 2

THM Modeling and Simulation of Circulation Tests for Optimized Development at the Utah FORGE Site

Robert Podgornery (Idaho National Laboratory)

The Utah FORGE (Frontier Observatory for Research in Geothermal Energy) project is at the forefront of advancing enhanced geothermal systems (EGS) through site development, innovative testing, and numerical modeling. This presentation will focus on the Thermal-Hydraulic-Mechanical (THM) modeling efforts, insights from recent circulation tests, and the overall site development timeline, with a special emphasis on the utilization of the FALCON code. Over the past several years, the FORGE project has undertaken extensive data collection and characterization activities, including the drilling, completion, and stimulation of long offset subhorizontal wells, and subsequent interwell circulation confirmatory testing. These efforts have provided critical data to continuously refine the conceptual and numerical models of the reservoir.

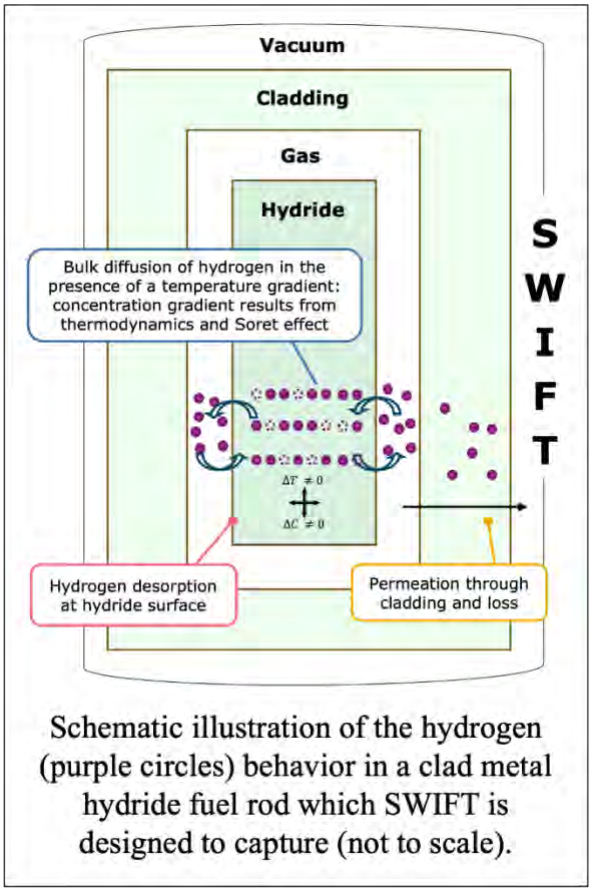
The THM models are essential for simulating the coupled responses of the subsurface to various FORGE activities, enabling accurate predictions of reservoir behavior and guiding experimental designs. Interwell circulation tests, conducted in 2023 and 2024 have been pivotal in developing and calibrating the THM simulation models. These tests have helped in adjusting the spatial and temporal reservoir properties to match observed pressure and production profiles, thus enhancing the reliability of the models. Key findings from these tests have prompted reevaluation of certain aspects of the discrete fracture network and early-time pressure data, leading to significant model improvements. The site development timeline for FORGE has been strategically planned to integrate continuous data collection, model refinement, and experimental validation. This iterative approach ensures that each phase of development builds upon the insights gained from previous activities, fostering a robust understanding of the reservoir dynamics.

NUCLEAR 4

Simulating Hydrogen Evolution in Metal Hydrides Using SWIFT

William Neilson (Los Alamos National Laboratory, LANL), Kai Duemmler (LANL), Christopher Matthews (LANL)

Hydrogen-based nuclear fuels combine neutron moderation with the fissile material and enable a reduction in the fuel mass or the required uranium enrichment in reactor designs. As such, they are pursued for use in special nuclear reactors, particularly where light weight and size are important for improved transportability (to space or other remote locations) and where highly enriched uranium is not desirable. A critical design and safety consideration in these reactors is the behavior of hydrogen. Hydrogen release, and its redistribution in the when fuel subjected to significant gradients in temperature, must understood and judged safe under normal operating conditions as well as under transient or accident conditions. Hydrogen behavior within an interconnected system (fuel, gas gap, and cladding) results in coupled nonlinear behavior that is nontrivial to compute. The MOOSE-based SWIFT tool (Stoichiometry With Internally Fluctuating Temperature) has been developed to tackle this problem. Utilizing the material properties of the metal hydride under consideration and the operating environment and conditions it resides in, the evolution of hydrogen under operating and accident conditions can be predicted.



Schematic illustration of the hydrogen (purple circles) behavior in a clad metal hydride fuel rod which SWIFT is designed to capture (not to scale).

Model of Hydrogen Corrosion of Nuclear Thermal Propulsion Carbide Fuel Using SWIFT

Kai Duemmler (Los Alamos National Laboratory, LANL), Christopher Matthews (LANL), Erofili Kardoulaki (LANL), Michael W.D. Cooper (LANL)

Nuclear thermal propulsion (NTP) is an alternative to the current chemical propulsion that has a higher specific impulse which will allow for human transportation to Mars, rapid cis-lunar transportation, or deeper into the solar system. In this work, the fuel and material interaction with hydrogen is studied using the finite element code Stoichiometry With Internally Fluctuating Temperatures (SWIFT), which is built on the Multiphysics Object Oriented Simulation Environment (MOOSE) framework. SWIFT couples the surface reactions (hydrogen corrosion and volatilization), the bulk diffusive behavior and heat transfer to model the hydrogen interaction with the solid solution carbide fuel. This will allow another avenue to interpret existing hydrogen exposure experiments in the existing literature. This will be a useful tool to for optimizing fuel composition and stoichiometry.

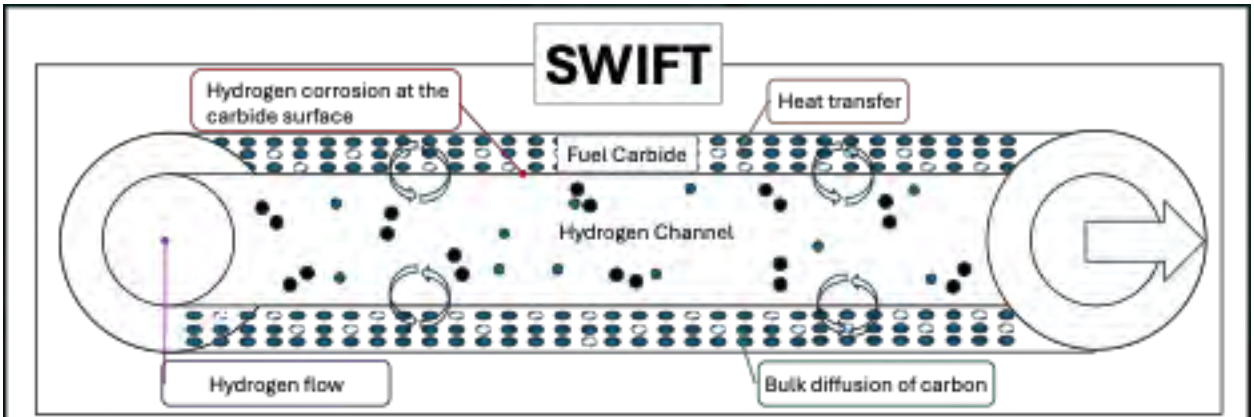


Fig. 1: Schematic of the NTP hydrogen (black) flow channel through the carbide fuel causing hydrogen corrosion of the carbon (blue) (not to scale).

Centipede: A MOOSE-Based Cluster Dynamics Code to Connect Lower-Length Scale Data to Fuel Performance Simulations

Christopher Matthews (Los Alamos National Laboratory, LANL), Michael Cooper (LANL), David Andersson (LANL)

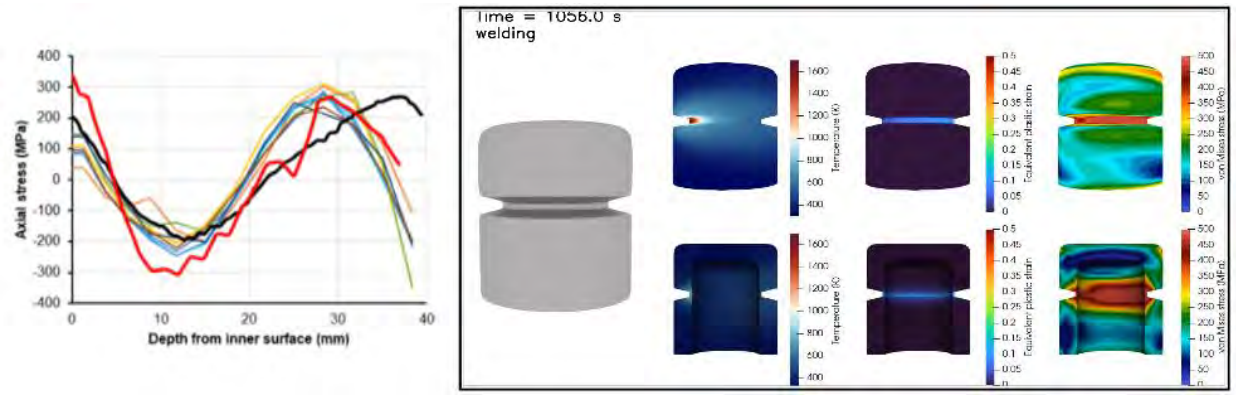
The diffusion of defects - both intrinsic defects like interstitials and vacancies, and fission products like xenon and zirconium - drives much of the unique behavior of nuclear fuel under irradiation. This includes behavior such as fission gas release and swelling, creep, and constituent redistribution, each of which contributes in non-trivial ways to the overall behavior of the fuel. Since diffusive mass flux itself is a well understood phenomenon, the behavior of these defects can be shown to be dependent on the individual species themselves, namely, their stability and mobility. Combined with terms for sources and sinks, rate theory or cluster dynamics tools can be used to predict the net diffusivity of defects. Unfortunately, these simple properties are difficult to extract for data-poor nuclear fuels. In particular, the high rate of damage accumulated by fission products during irradiation creates a complex environment, and thus, a highly non-linear computational problem. In order to predict the behavior of defects during irradiation in nuclear fuel, the cluster dynamics code Centipede was developed at Los Alamos National Laboratory. Since it is based on the MOOSE framework, Centipede benefits from the native non-linear solvers in MOOSE, as well as natural coupling to engineering scale (e.g., BISON) and data science codes. In addition, by leveraging lower-length scale computational data, cluster dynamics simulations can serve as the missing link between the atomistic and engineering scales. We will show how Centipede has been able to quantitatively compare to experimental data on fission gas diffusivity, how it can be easily extended to fuels that lack data, and how it can be coupled to BISON and stochastic tools to show uncertainty quantification for engineering scale problems.

Three-Dimensional Welding Simulation of a Pressure Vessel and Validation Against UK R5 Procedure

Bipul Barua (Argonne National Laboratory, ANL), Tianchen Hu (ANL), Mark Messner (ANL)

Residual stresses induced by welding processes can significantly affect the structural integrity and performance of welded components used in nuclear reactors. Accurate determination of these stresses is crucial for predicting various failure modes, such as stress relaxation cracking (SRC) and Type IV cracking, optimizing welding procedures, and extending the service life of structures. This study presents a comprehensive finite element analysis (FEA) approach using the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework to determine residual stress distributions in welded components. Thermal and mechanical phenomena associated with the welding process were simulated by coupling heat transfer and elastic-plastic-creep deformation models within MOOSE. A three-dimensional FEA model of a welded vessel example from the UK's nuclear Code R5 was developed, incorporating an ellipsoidal moving heat source in MOOSE to represent the welding arc and temperature distribution during welding. The model utilized MOOSE's Element Subdomain Modifier to add elements at the joint, representing the progressive addition of weld material as welding progresses - a capability not available in commercial software. Most weld simulations in the literature using commercial software introduce all filler material in a weld pass instantly and then move the heat source to simulate temperature and resulting thermal stress. In contrast, our simulation framework allows for the continuous addition of filler material as the heat source moves, providing a more realistic representation of the welding process, which is reflected in the variation of through-thickness stress at different circumferential locations. The coupled thermal-structural simulation then calculated the welding residual stresses after the vessel cooled to room temperature. The residual stresses were verified against experimental measurements provided in R5, obtained using deep-hole drilling techniques. The comparison demonstrated that the MOOSE-based FEA accurately predicted the residual stress profiles,

showing good agreement with experimental data. This study highlights the effectiveness of MOOSE in handling complex multiphysics problems in welding simulations and provides insights into the influence of welding parameters on residual stress formation. The findings underscore the importance of advanced simulation tools in assessing residual stresses and offer a pathway for design assessment of nuclear reactor welded components concerning weld residual stress-related failure modes, as well as optimizing welding processes to minimize detrimental stress concentrations.

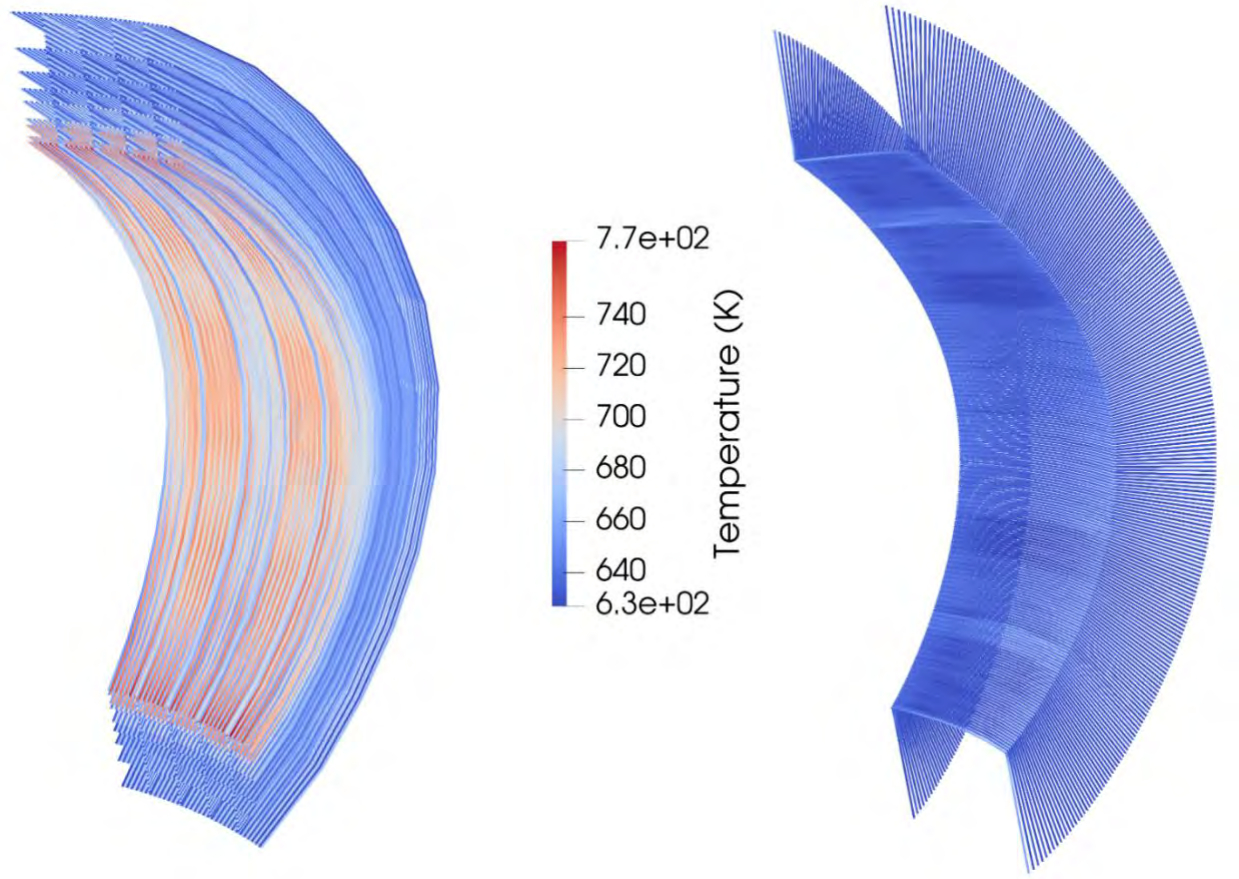


FUSION 2

New Developments and Verification of Fusion Blanket Simulation Capabilities in the MOOSE Framework

Trevor Franklin (Virginia Commonwealth University, VCU), Casey Icenhour (Idaho National Laboratory, INL); Pierre-Clement A. Simon (INL), Paul Humrickhouse (Oakridge National Laboratory), Fande Kong (INL, at time of contribution), Lane Carasik (VCU)

Multiphysics modeling capabilities have a crucial role to play in the accelerated deployment of fusion energy. To that end, we developed new multiphysics fusion blanket simulation capabilities in the Multiphysics Object-Oriented Simulation Environment (MOOSE). Our contribution is threefold. Firstly, we expanded existing capabilities, including thermal hydraulics, fully three dimensional (3D) heat transfer, and integrated neutronics analysis by coupling 3D tritium transport modeling capabilities using the Tritium Migration Analysis Program, version 8. Secondly, we performed a thorough verification of the new capabilities and increased testing code coverage to meet MOOSE's software quality standards. The MOOSE framework follows a strict software quality assurance plan to be Nuclear Quality Assurance, Level~1 compliant. The new multiphysics fusion blanket simulation capabilities are now held to the same standard. Thirdly, to demonstrate MOOSE's new fusion blanket modeling capabilities, we performed a fully integrated, multiphysics simulation of a 3D solid ceramic breeder blanket design. This proof-of-concept simulation provides the temperature and tritium distribution across the blanket. The combined efforts towards software quality and the development of multiphysics coupling capabilities provide an effective and reliable framework for modeling solid ceramic fusion blankets using MOOSE.



Fusion Energy System Liquid Immersion Blanket System Modeling using SAM

Lane Carasik (Virginia Commonwealth University, VCU), Trevor Franklin, (VCU), Ryan McGuire (VCU), Sierra Tutwiler (VCU)

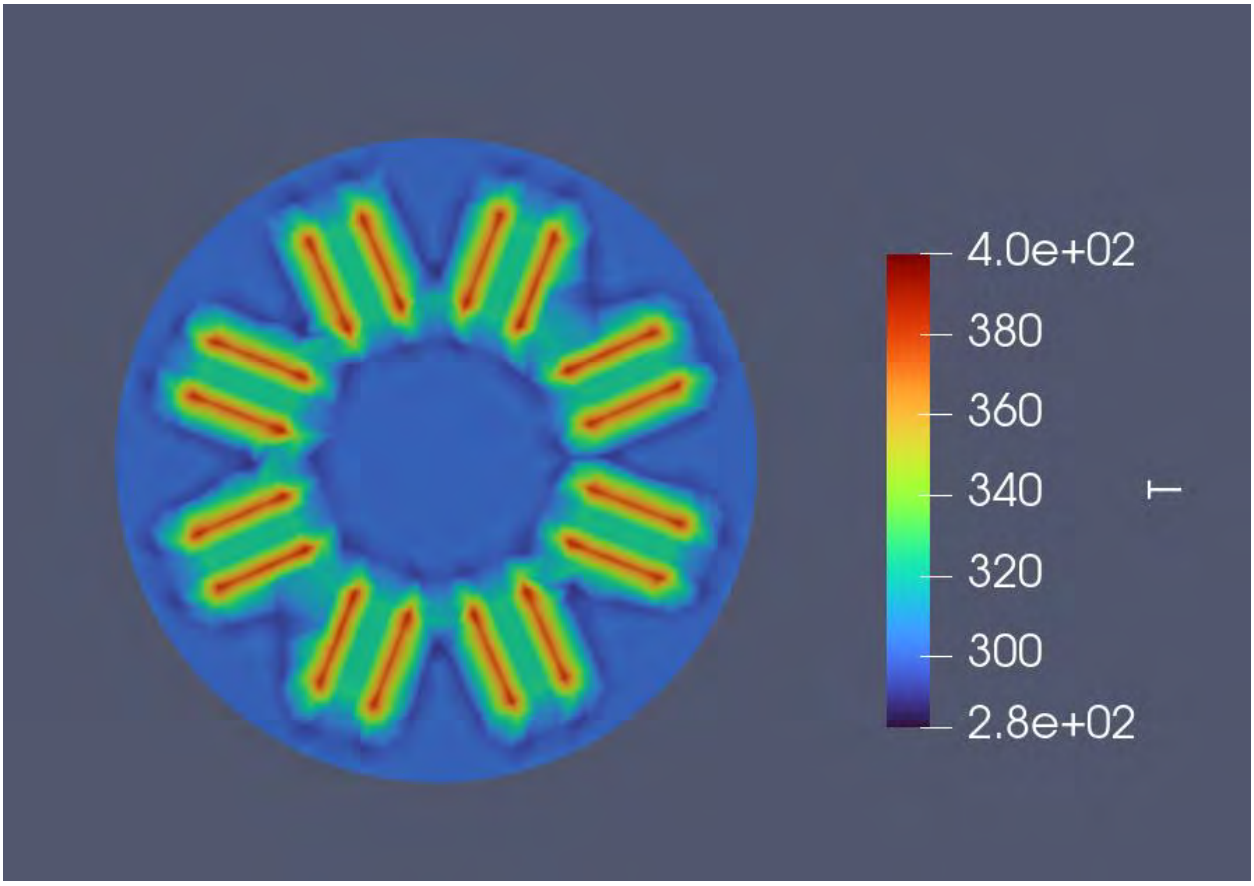
As the push to deploy fusion energy systems continues through public and commercial initiatives, the determination of the design and accident scenarios figures of merit with the highest influence on design and safety is required. Current fusion energy system designs involve either solid or liquid blanket systems that serve the purpose of tritium (fuel) management, neutron multiplication, and heat removal for power conversion. One concept, involving the use of fluoride based molten salts in fusion breeder blankets has become a potential option. This is the Affordable, Robust, and Compact (ARC) energy system that involves a liquid immersion blanket (LIB) design for fuel cycle and heat management. LIBs involve a molten salt (i.e. FLiBe) as the working fluid, coolant, and fuel source in the heat transport system that removes heat from the plasma facing components and blanket components. At the time of writing, a significant gap exists in both systems and component level information for LIBs needed for open-source research and development of different enabling technologies. To address these gaps, the authors have investigated FLiBe based LIBs using system & component modeling with MOOSE based tools and experimental investigations. The modeling work involves using the Department of Energy's MOOSE based System Analysis Module (SAM) code developed by Argonne National Laboratory. Leveraging the capabilities for modeling molten salt

reactors in SAM, the system behavior of a prototypical ARC LIB has been analyzed for start-up, shutdown, steady state, and pump failure transients for the heat transport systems. For each scenario, the potential for structural failure of plasma facing components and heat transport system components is analyzed to determine inappropriate design choices. In the reported work, we will discuss both operational transients and accident scenarios modeled using SAM and how future coupling with MOOSE tools will be useful for fusion energy system design. Additionally, the authors will discuss how the data produced from this study has provided a foundation for component level studies using other DOE NEAMS tools and experiment methodologies.

MOOSE Model of the LOBO Lead Loop

Son Quang (University of Tennessee, Knoxville, UTK), Nicholas Brown (UTK), G. Ivan Maldonado (UTK)

The Lobo Lead Loop (LLL) at the University of New Mexico (UNM) is a unique platform for investigating the corrosive effects of molten lead. As the only forced convection pure lead loop in the U.S., the LLL provides invaluable experimental data for validating computational models. This study leverages the Thermal Hydraulic Module (THM) within the MOOSE framework to simulate the complex fluid dynamics and heat transfer processes within the LLL. By replicating the loop's geometry and operational conditions, we aim to benchmark MOOSE's predictions against experimental data. This validation is crucial for assessing the code's ability to accurately model lead-lithium behavior, a promising tritium breeding material for Dual Coolant Lead Lithium (DCLL) fusion reactor blankets. An accurate representation of liquid lead's thermophysical properties, including density, specific heat capacity, thermal conductivity, and viscosity, is essential for realistic simulations. These properties vary with temperature, significantly influencing the fluid's behavior under different operating conditions. Additionally, careful consideration of boundary conditions, such as inlet/outlet flow rates, pump pressure, and heat fluxes, is necessary to mimic the experimental setup. To accurately predict temperature distributions, the simulation must account for all relevant heat transfer mechanisms, including convection and radiation. These mechanisms interact and influence the overall thermal behavior of the system. By comparing the simulated temperature and pressure drop with results from the RELAP5-3D model of the LLL, we can evaluate MOOSE's capability to accurately model the system's behavior. The current LLL doesn't have a magnetic field in the specimen test section for magnetohydrodynamic (MHD) related studies. The new LLL being established with the magnetic field (1-2T) will have the capability to conduct MHD studies. Future work will involve using the MOOSE framework to simulate the behavior of the new LLL, which will include a magnetic field for MHD studies. The MOOSE's modules, such as THM, Heat Transfer, Electromagnetics, etc., will be used to perform predictive simulations of the new LLL.

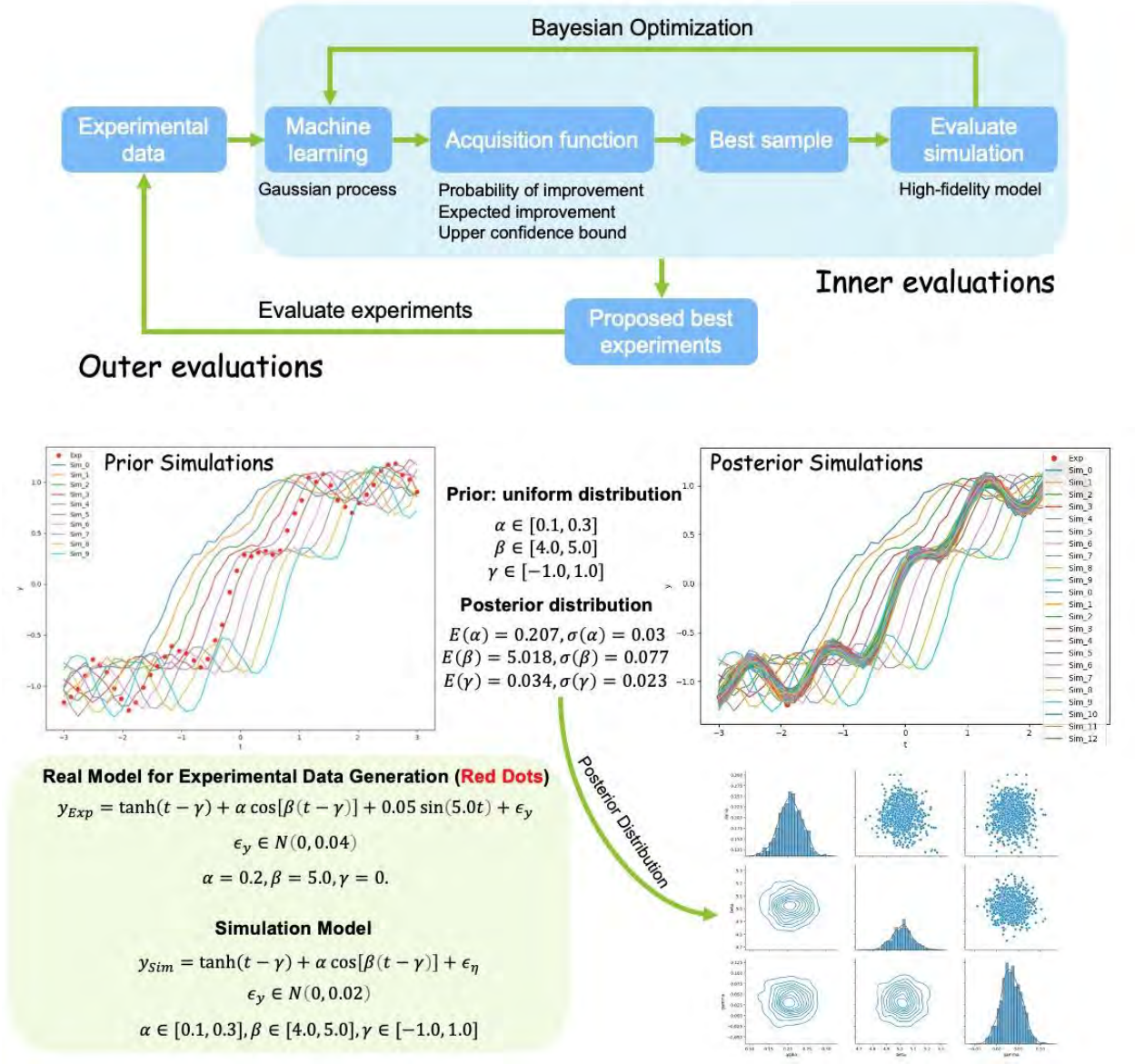


NUCLEAR EXPERIMENTAL DESIGN 2

Platform of Optimal Experiment Management via RAVEN and MOOSE to Accelerate the Discovery of Optimal Solutions

Congjian Wang (Idaho National Laboratory)

POEM is a platform for optimal experiment management, powered with automated machine learning to accelerate the discovery of optimal solutions, and automatically guide the design of experiments to be evaluated. POEM currently supports 1) random model explorations for experiment design, 2) sparse grid model explorations with Gaussian Polynomial Chaos surrogate model to accelerate experiment design ,3) time-dependent model sensitivity and uncertainty analysis to identify the importance features for experiment design, 4) model calibrations via Bayesian inference to integrate experiments to improve model performance, and 5) Bayesian optimization for optimal experimental design. In addition, POEM aims to simplify the process of experimental design for users, enabling them to analyze the data with minimal human intervention, and improving the technological output from research activities. POEM leverages RAVEN (a robust platform to support model explorations and decision making) and MOOSE to allow for large scalability and reduction of the computational costs and provides access to complex physical models while performing optimal experimental design.

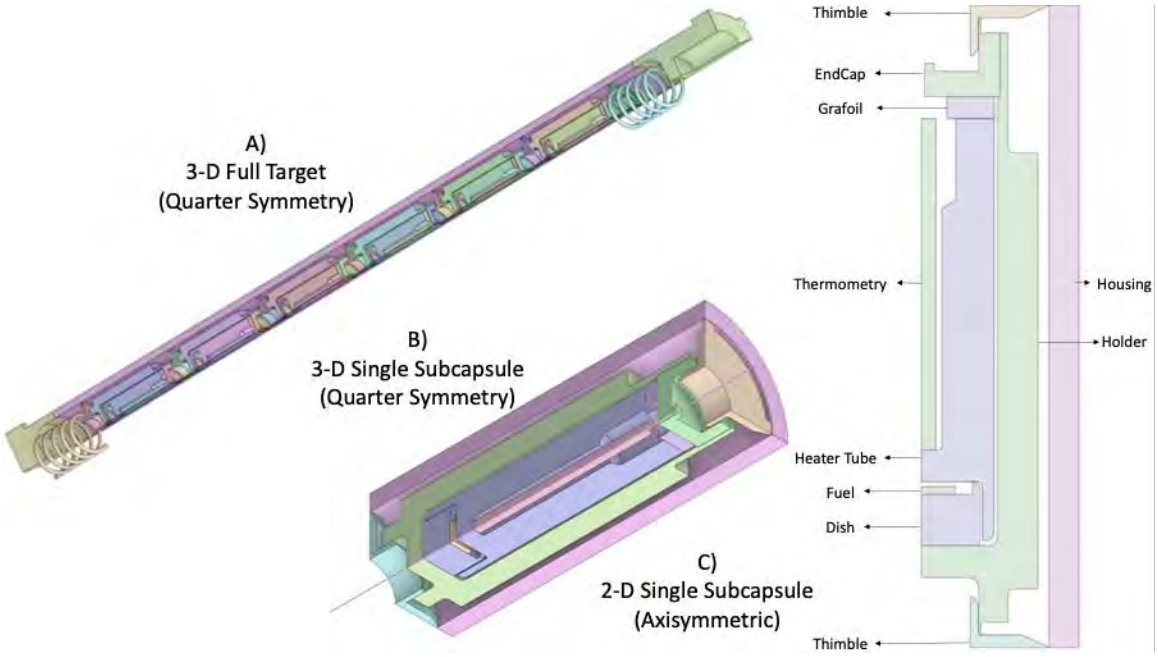


Assessing Influence of Fission Gas Release in MiniFuel Irradiation Capsule Design

Nicholas Meehan (University of Tennessee Knoxville, UTK), Jacob P. Gorton (Oak Ridge National Laboratory), Nicholas R. Brown (UTK)

The MiniFuel irradiation platform at Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR) is a flexible, high-throughput separate effects test capability for accelerated burnup. MiniFuel irradiation capsules contain a miniature fuel compact; small enough that fission within the fuel is not the main source of heating. Instead, gamma heating from the surrounding metallic components provides the majority of the heat to the fuel. This allows the MiniFuel design to isolate fuel irradiation temperature from fission rate, facilitating irradiation at constant temperatures. Data from these experiments can be used to inspect specific operational regimes of candidate fuels and to develop models for irradiation effects. Finite element thermal models within ANSYS are relied

upon to design MiniFuel experiments and to achieve experimental objectives. MiniFuel capsules do not contain in-situ measurement tools, so information is gathered during post-irradiation examination. A passive thermometry rod made is used to determine the irradiation temperature and the fuel and capsule fillgas are analyzed following irradiation. A recent study on the model predictions revealed that there is uncertainty stemming from the thermal contact conductance predictions within the ANSYS model. One of the main drawbacks to the ANSYS model is that it does not consider fission gas release, which can have significant impact on the thermal conductivity of the capsule fillgas. To understand this uncertainty, we have developed a model within BISON which has a robust fission gas release model. For a consistent comparison with ANSYS, we will be implementing the thermal contact conductance model from the ANSYS MiniFuel model into BISON. We can then perform a sensitivity analysis on the model inputs to quantify the influence of fission gas release on the temperature prediction of the fuel. This study will showcase the use of the BISON code framework to analyze fission gas release and gap heat transfer.



Development of Copper Corrosion Simulation Code for Performance Assessment of Deep Geological Repository Systems: HADES (High-level rAdiowaste Disposal Evaluation Simulator)

Pilhyeon Ju (Seoul National University, SNU), Nakkyu Chae (Co-first Author) (Korea Atomic Energy Research Institute), Samuel Park (SNU), Seongkoo Hong (SNU), Sungyeol Choi (Corresponding Author) (SNU & Nuclear Research Institute for Future Technology and Policy & Institute of Engineering Research)

For the safe disposal of Spent Nuclear Fuel (SNF) from the environment, a Deep Geological Repository (DGR) should be built to prove a barrier system and validated via performance assessments. This study, which developed a new multi-physics simulation code called HADES (High-level rAdiowaste Disposal Evaluation Simulator), covers THC-EC (Thermal-Hydraulic-Chemical-Electrochemical) multi-physics of deep geological environment by using the MOOSE

framework. To quantify the integrity of copper canisters used in DGRs, corrosion behavior at the copper surface should be understood to ensure that the canister safely endures against the failure due to corrosion during its service time. Here, the developed HADES code focuses on the uniform corrosion of copper, thereby calculating the estimated depth of the corrosion at the copper canister surface. The basic structure of HADES is a multi-app system, with the main application solving THC behaviors and the sub application calculating the EC behavior regarding uniform corrosion of copper. In every single time step, the sub application solves the six reactions related to the copper corrosion, all of which are expressed in the form of Bulter-Volmer Equation. The Mixed Potential Theory is used to calculate the corrosion potential numerically, the value of which is determined in the point where the sum of corrosion currents from the six reactions become zero. With the derived corrosion potential, HADES can calculate the amount of corrosion products and the depth of corrosion. Copper corrosion results calculated using HADES were validated by comparing to the experiment results published by Professor David W. Shoesmith's Team; the calculated corrosion potential and film thickness showed a similar scale and behavior with the experimental results. Also, laboratory-scale experiments for corrosion potential were performed in oxic and anoxic environments to validate the results from the simulation code. The experiment results from both environments showed similar behaviors, with the various conditions of temperature, concentration of HS- and Cl-, and pH being validated. The HADES uniform corrosion code is now utilized in describing the estimated Korean disposal environment. The calculated average corrosion rate of the Korean disposal concept corresponded to 0.05 Î¼m/yr. The simulation code was improved in order to consider Cu(I) and FeS2 oxidation with Arrhenius Equations, and the simulation result shows that the copper canister will be corroded by about 29 mm during 1 million years, in a conservative assumption that HS- would be continuously supplied to the environment. The radiolysis reactions are also reflected, with the results showing that the corrosion depth by radiolysis product would be about 23 Î¼m and a corrosion potential of between -0.4 ~ -0.7 V_SCE. With these results, the HADES simulation code is expected to have a key role in calculating the uniform corrosion of copper canisters in diverse DGR environments.

SPECIAL TOPICS 3

Concurrent Multiscale Simulations of Nonlinear Random Materials using Probabilistic Learning

Peiyi Chen (The AI Institute), Johann Guilleminot (Duke University), Tianchen Hu (Argonne National Laboratory)

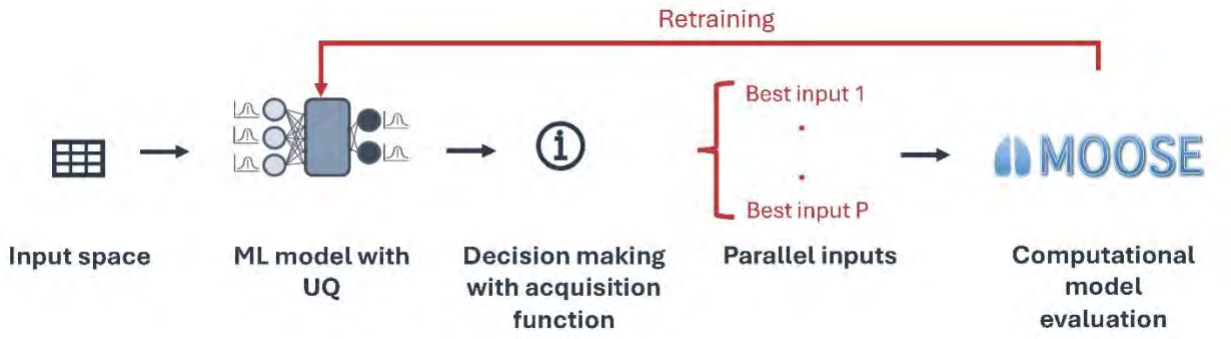
This work is concerned with the construction of statistical surrogates for concurrent multiscale modeling in structures comprising nonlinear random materials. The development of surrogates approximating a homogenization operator is a fairly classical topic that has been addressed through various methods, including polynomial- and deep-learning-based models. Such approaches, and their extensions to probabilistic settings, remain expensive and hard to deploy when the nonlinear upscaled quantities of interest exhibit large statistical variations (in the case of non-separated scales, for instance) and potential non-locality. The aim of this paper is to present a methodology that addresses this particular setting from the point of view of probabilistic learning. More specifically, we formulate the approximation problem using conditional statistics, and use probabilistic learning on manifolds to draw samples of the nonlinear constitutive model at mesoscale. Two applications, relevant to inverse problem solving and forward propagation, are presented in the context of nonlinear elasticity. We show that the framework enables accurate predictions (in probability law), despite the small amount of training data and the very high levels of nonlinearity and stochasticity in the considered system.

MOOSE ProbML: Parallelized Probabilistic Machine Learning and Uncertainty Quantification for Computational Models

Somayajulu L N Dhulipala (Idaho National Laboratory, INL), Peter German (INL), Xianjian Xie (Arizona State University), Zachary Prince (INL), Yifeng Che (INL), Vincent Laboure (INL)

The Multiphysics Object Oriented Simulation Environment (MOOSE) is a widely used open-source finite element software for performing multiphysics multiscale simulations in a massively parallel fashion. Recently, the computational team at Idaho National Laboratory (INL) has implemented Probabilistic Machine Learning (ProbML) capabilities in MOOSE -in a parallelized fashion- and enable active learning with large-scale computational models for tasks such as surrogate model development, scale bridging, forward/inverse uncertainty quantification (UQ), Bayesian optimization, etc. This presentation summarizes these developments in MOOSE along with demonstrations on several real applications relevant to nuclear energy. At the fundamental level, samplers like Monte Carlo/Latin Hypercube, variance reduction, parallelized Markov Chain Monte Carlo (MCMC) support uncertainty propagation in both forward and inverse settings. These samplers can be integrated with the Gaussian processes (GP) suite in MOOSE, which offer several variants like scalar GPs, multi-output GPs, and deep GPs, to enable active learning. These GPs can be tuned using gradient-based optimization methods like Adam and its variants or gradient-free methods like the elliptical slice sampler (a variant of MCMC adept under Gaussian settings) for more complex covariance kernels or likelihoods whose gradient computations can be cumbersome. A variety of batch acquisition functions permit parallelized evaluation of the computational model and support different learning objectives with high efficiency like Bayesian

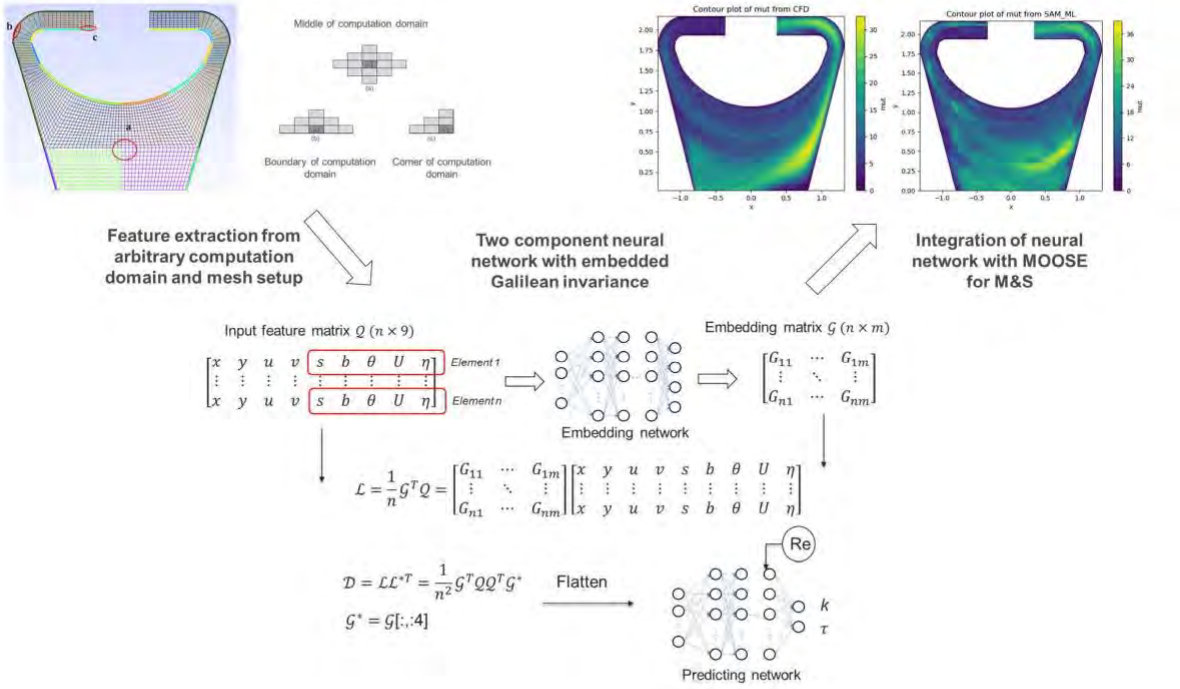
inference, global surrogate development, optimization, etc. Furthermore, libtorch integration supports training, evaluation, and re-training of neural networks and other complex machine learning models in active learning settings. The impacts of these developments are shown on several real applications: (1) nuclear fuel inverse UQ and model inadequacy assessment using the Kennedy O'Hagan framework; (2) uncertainty aware surrogate modeling for additive manufacturing to predict field quantities; (3) nuclear reactor rare events analysis; and (4) complex fluid flow prediction using a global surrogate with quantified prediction uncertainty. Finally, the outlook of MOOSE ProbML is discussed for both outer-loop and inner-loop computations in the broad view to accelerate fuels and materials qualification, address gaps in knowledge and data, and assess new reactor/fuel systems.



A Galilean-Invariant Neural Network Closure for Enhanced Turbulence Modeling in MOOSE-Based Nuclear Thermal-Hydraulics Simulation

Yang Liu (Texas A&M University)

This work presents the development of a novel neural network architecture embedded with Galilean invariance, specifically designed to enhance the modeling capabilities of the MOOSE Navier-Stokes module for nuclear thermal hydraulics applications. The neural network functions as a data-driven eddy viscosity closure, enabling accurate turbulence modeling across a variety of geometric configurations and mesh structures. Trained on high-fidelity computational fluid dynamics (CFD) data, the neural network predicts local eddy viscosity based on flow features from adjacent regions, maintaining reliable performance across diverse flow conditions. The model's incorporation of Galilean invariance allows for its application to irregular computational domains, making it particularly suitable for simulating complex fluid dynamics in advanced reactors, such as liquid-fueled molten salt reactors (MSRs). Additionally, the use of non-dimensional inputs enhances the network's flexibility, facilitating interpolation and extrapolation across different Reynolds numbers within the fully turbulent flow regime. The integration of this neural network with the MOOSE Navier-Stokes module demonstrates improved accuracy and efficiency in thermal-fluid simulations. The results align closely with high-fidelity CFD benchmarks, indicating the potential of this approach to support the safety analysis and design of advanced nuclear reactors. This integration addresses the challenges posed by complex geometries and turbulent flow conditions in next-generation nuclear reactor designs.



Controller Training with Reinforcement Learning in MOOSE

Peter German (Idaho National Laboratory, INL), Dewen Yushu (INL)

Reinforcement Learning (RL), as a rapidly evolving branch of Artificial Intelligence (AI) and Machine Learning (ML), has been successfully deployed in the field of robotics, and has been intensively researched for the optimal control of autonomous devices such as cars or drones. The training of the controllers necessitates repeated interactions between an agent and the environment. Although some applications, such as the control of robotic arms or drones, allow training using real-world equipment, many applications rely on specifically chosen virtual training environments. In these cases, the agent interacts with a virtual space that simulates the expected responses for given actions. For many applications, these virtual training environments can greatly accelerate the training process and reduce material costs. Recently, the Multiphysics Object-Oriented Simulation Environment (MOOSE) has been extended with interfaces to the C++ front end of Pytorch to support of machine learning applications within MOOSE. These capabilities together with the already existing MultiApp and Control systems of MOOSE have been harnessed for the training and research of smart controllers for multiphysics problems. This presentation discusses the current status of deep reinforcement learning capabilities in MOOSE along with various demonstrative examples such as the temperature control in a room or the control of a melting process using a laser beam.

Wednesday, March 12

PLENARIES

Using MOOSE to Investigate Material Behavior in Harsh Environments

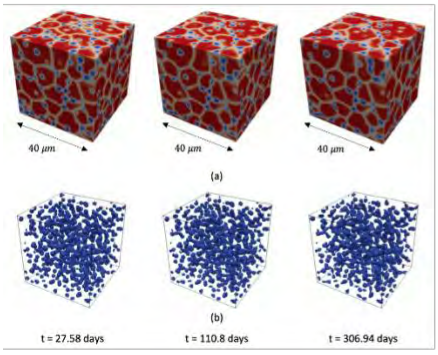
Mike Tonks (University of Florida, UF), Ali Muntaha (Purdue University), Sourav Chatterjee (Lawrence Livermore National Laboratory), Chaitanya Bhave (Idaho National Laboratory), Thompson Igunma (UF), Soumya Bandyopadhyay (UF), Marina Sessim (QuantumScape), Robert Clayton (UF), David Andersson (Los Alamos National Laboratory), Brian Wirth (University of Tennessee-Knoxville, UTK), Sophie Blondel (UTK)

Understanding material behavior in harsh environments is essential for advancing technologies in nuclear energy, aerospace, and other high-performance applications. The materials tetrahedron—structure, processing, properties, and performance—provides a foundational framework for materials science, but it becomes highly dynamic in harsh environments, where these properties evolve continuously during operation. This complexity makes experimental investigation both expensive and technically challenging, highlighting the critical role of computational modeling in probing material behavior under such conditions. The Multiphysics Object-Oriented Simulation Environment (MOOSE) is particularly well-suited for modeling materials in harsh environments due to its flexibility, ability to couple multiple physics, scalability across length scales, and compatibility with high-performance computing. In this presentation, we will showcase how MOOSE facilitates advanced simulations in harsh environments through three compelling examples:

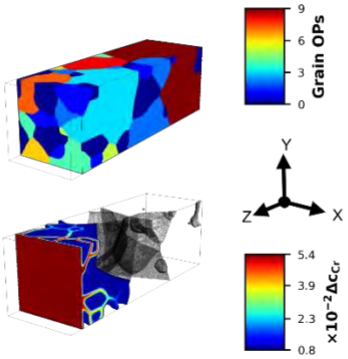
1. Fission gas bubble evolution and release, using a coupled cluster dynamics and phase field model.
2. Molten salt corrosion and solid-state batteries, exploring degradation mechanisms and electrochemical interactions in extreme chemical environments.
3. Ablative thermal protection systems for atmospheric entry, simulating coupled mass loss, heat transport, and endothermic chemical reactions.

These examples demonstrate the versatility of MOOSE in addressing multidisciplinary challenges and its capacity to drive innovation in materials science for harsh environment applications.

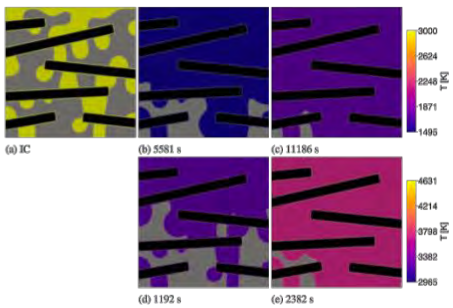
Fission Gas Bubble Evolution



Corrosion Due To Molten Salt



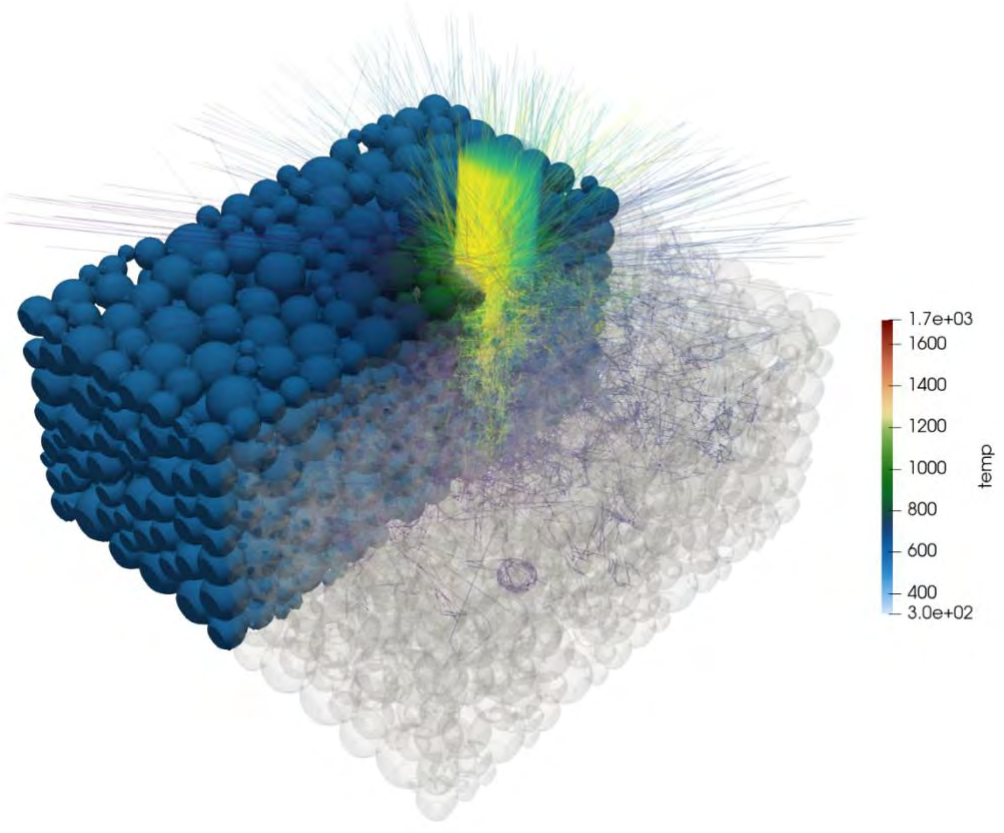
Thermal Protection System Ablation



Multiphysics Modeling of the Additive Manufacturing Process Using the MOOSE framework

Wen Jiang (North Carolina State University), Dewen Yushu (Idaho National Laboratory)

There is significant interest in high-fidelity process modeling for additive manufacturing (AM) techniques. Modeling and simulation can provide the insight for a rational design by addressing the basic science and engineering needs for AM process, leading to a mechanistic understanding of processing-structure-property relationships, which are fundamental to design and develop innovative fabrication techniques. At mesoscale, a high-fidelity numerical model including heat transfer, fluid flow and mass transport, is developed in MALAMUTE (MOOSE Application Library for Advanced Manufacturing UTilitiEs) to simulate the melt pool physics. Ray-tracing capability in MOOSE is leveraged to accurately tract the interaction between powder addition and laser heat source. The temperature, chemical composition and solidification rate of melt pool can be predicted and thereafter used in lower-length scale model to simulate microstructure evolution.



Modeling and Simulation of the eVinci Microreactor Using MOOSE-Based Tools

Kallie Metzger, Westinghouse Electric Company

This presentation provides a description of the eVinci microreactor and its analysis approach using MOOSE-based tools, focusing on both steady-state and transient safety scenarios. The analysis

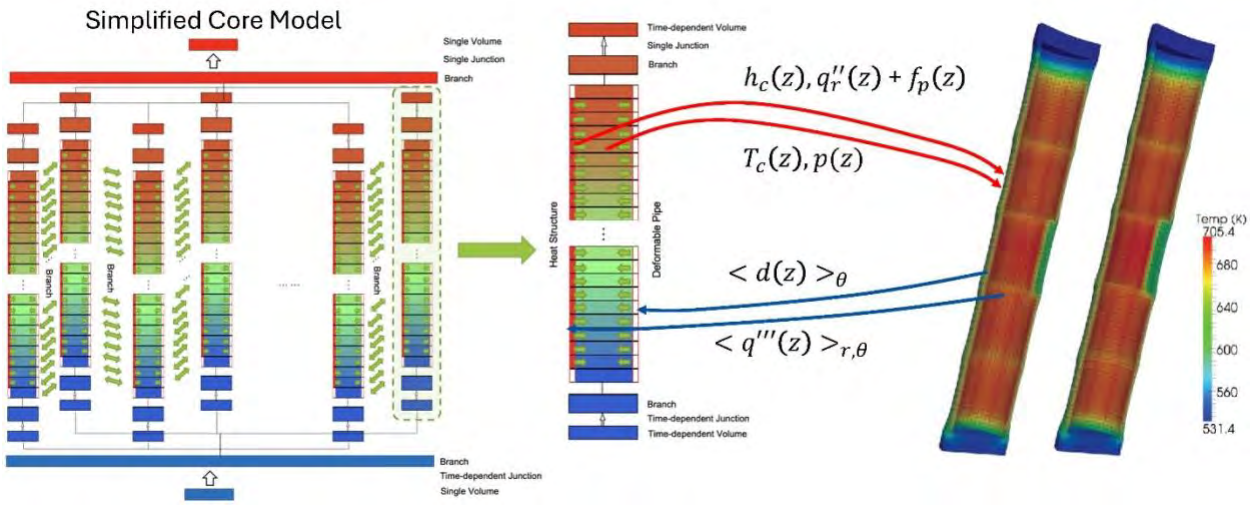
methodology employs a suite of coupled multiphysics codes, including Griffin for neutron transport, Bison for fuel performance, and the MOOSE Thermal-Hydraulic Module for modeling the secondary-side air flow to accurately capture the reactor's behavior under various operational conditions. A critical component of the analysis framework is the TRISO fuel performance analysis, which ensures the robustness and reliability of the fuel under normal and abnormal conditions. Through detailed simulation and modeling, this work aims to provide valuable insights into the safety margins and operational efficiency of the eVinci Microreactor, paving the way for its potential deployment in diverse energy applications.

NUCLEAR 5

In Memory Coupling of BISON and RELAP5-3D to Simulate LOCA Behavior in LWRs

Kyle A. Gamble (Idaho National Laboratory), Ken Yueh (Electric Power Research Institute)

Large-scale light-water reactor nuclear power plants have been in operation for several decades in the United States. To improve the economics of these plants the industry is seeking regulatory approval to increase the discharge burnup and enrichment of the fuel used in these plants to increase cycle length and reduce refueling costs. Experimental evidence from several international programs indicates that as the burnup increases there is the potential for fuel fragmentation, relocation, and dispersal (FFRD) to occur during a Loss of Coolant Accident (LOCA). The onus falls to the fuel vendors to demonstrate that FFRD can be mitigated or is a non-issue based upon LOCA studies of high burnup core designs. The Electric Power Research Institute (EPRI) and Idaho National Laboratory have partnered through a US Department of Energy Technology Commercialization Fund project to develop a LOCA analysis tool for adoption by industry in support of their efforts. The LOCA analysis tool couples the BISON fuel performance code and RELAP5-3D together in memory for improved LOCA modeling capabilities. The project consists of four main development areas: BISON developments, BISON-RELAP5-3D coupling, verification and validation, and best-estimate plus uncertainty. The BISON areas of development focus on partial axial fuel relocation, axial gas communication, cladding ballooning and burst, and multi-rod analyses. Coupling activities are concerned with ensuring proper information flow in memory between BISON and RELAP5-3D and achieving conservative transfers between the codes. Verification proves proper coupling for standard problems whereas validation demonstrates the improvement in fuel performance and thermal-hydraulic predictions to experiments versus using the individual codes by themselves. The best estimate plus uncertainty capability leverages stochastic tools module available through the Multiphysics Object-Oriented Simulation Environment (MOOSE). This talk will cover several aspects of the project, providing details on BISON improvements, the coupling strategy, and verification and validation cases including best estimate plus uncertainty on the results.



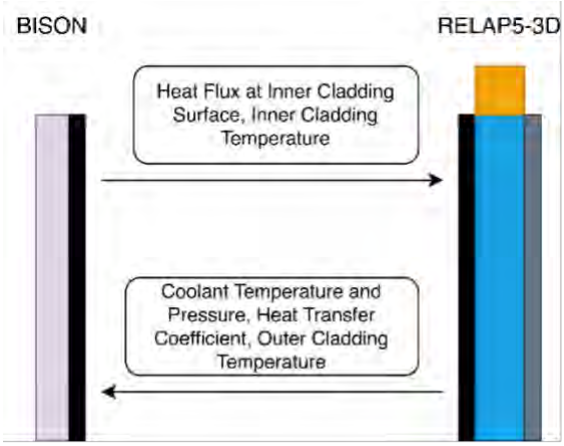
BISON and RELAP5-3D For Pressurized Water Reactor Safety Applications

Mason A. Fox (University of Tennessee, Knoxville, UTK), Nicholas R. Brown (UTK)

Expanded capabilities provided by advanced modeling and simulation tools now enable previously unachievable fidelity and scale in reactor safety analysis. As the nuclear industry and research communities reimagine the role of nuclear power in meeting our infrastructure needs, more accurate reactor safety performance predictions are required. Well-validated computational models offer powerful capabilities for safety analysis and the identification of important factors that should be targeted for uncertainty reduction. The use of these tools in computational studies supports both an improved physical understanding of accident phenomena and potential cost reductions in reactor development and deployment. Two examples of safety analysis using both fuel performance and thermal-hydraulic modeling are discussed, demonstrating application of RELAP5-3D and BISON to design basis accident analysis, importance ranking of uncertain parameters for fuel-to-coolant heat transfer, and design screening of proposed high burnup pressurized water reactor designs.

1. A tightly coupled RELAP/BISON model was used to study reactivity-initiated accident pulses, focusing on the interaction between thermomechanical and two-phase thermal-hydraulic behavior and the consequences for fuel integrity. Results of these simulations indicate that the rate of heat transfer through the system and the system mechanical response both impact timing and severity of the event. Occurrence of critical heat flux, film boiling heat transfer, pulse width effects, pellet-cladding frictional contact, and many additional material factors were shown to be important. Further investigation and improvement of these models provide high value opportunities for improving code capabilities for rapid power transients.
2. Loosely coupled RELAP and BISON models were applied to explore the safety implications of high burnup fuels on loss of coolant accidents. The work focuses on the effects of introducing gadolinium burnable poisons as an alternative to boron-based Integral Fuel Burnable Absorbers (IFBA) in pressurized water reactors. Preliminary results suggest that gadolinia burnable absorbers are beneficial for reducing rod internal pressures and delaying cladding burst while still providing sufficient reactivity hold-down.

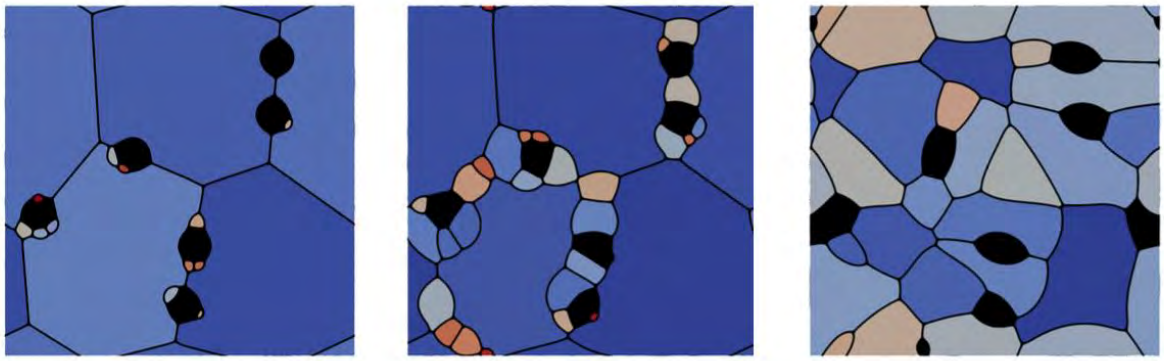
The two applications presented are examples of important use cases for BISON and RELAP5-3D. These tools have powerful capabilities for reactor safety analysis, can support experimentation by identifying high importance, high uncertainty model factors, and provide opportunities for improved theoretical understanding of accident behavior. Continued development of these tools will be essential to support the growth of the nuclear industry for power generation applications and the expansion of nuclear energy into new, socially beneficial domains.



Meso-Scale Modeling for Restructuring in the High Burnup UO2 Nuclear Fuel

Sudipta Biswas (Idaho National Laboratory, INL), Larry K. Aagessen (INL)

In this work, we utilize MOOSE and MOOSE-based application MARMOT, to simulate the microstructural evolution and restructuring observed in the high burnup UO2 nuclear fuel. This work realistically simulate the restructuring behavior observed in different regions of a high burnup fuel. We employ a grand-potential based phase-field model to concurrently evaluate the formation of subgrains and growth of fission bubbles within the fuel. A energy-based subgrain formation criteria is introduced to simulate the restructuring process. The effect of different initial conditions and different modeling parameters are studied systematically to capture how each of these parameters influence the characteristics of the restructured fuel. It is observed that the subgrain formation begins around existing fission gas bubbles and then proceeds towards triple junctions, grain boundaries and grain interiors. Different restructuring stages are shown in the following figure. The predicted microstructures are consistent with experimental observations of the restructured regions. Additionally, a correlation is presented to demonstrate the evolution of the restructuring volume fraction as a function of local effective burnup. This work provides a first of its kind mechanistics restructuring model that can be used by BISON for performance prediction of high burnup UO2 fuel.



Fission Gas Behavior Modeling in BISON for Fuel Performance Calculations

Pierre-Clement Simon (Idaho National Laboratory, INL), Lary K. Aagesen (INL), David Andersson (Los Alamos National Laboratory, LANL), Sudipta Biswas (INL), Nathan Capps (Oak Ridge National Laboratory), Michael W.D. Cooper (LANL), Kyle Gamble (INL), Christopher Matthews (INL), Steve Novascone (INL)

One of the first and widely used MOOSE-based applications is the fuel performance code BISON. BISON directly benefits from MOOSE's ability to perform complex multiphysics simulations and applies it to the field of nuclear fuel performance. Predicting nuclear fuel performance during normal operations and accident scenarios is crucial to ensure the safety and performance of fission nuclear reactors. Fission gases greatly influence fuel performance. The fission of nuclear fuel results in fission products with a fraction of them being noble gases due to low solubility. They diffuse through the fuel matrix and grain boundaries, join or form intra- and inter-granular bubbles, and eventually get released from the fuel into the fuel-cladding gap and rod plenum. Fission gas behavior is central to fuel performance because it degrades the rod thermal conductivity and mechanical behavior. The presence of fission gases within the fuel decreases its thermal conductivity and leads to fuel swelling, cracking, and pulverization, which can result in pellet-cladding interactions. Further, as fuel utilization increases, fuel microstructure evolves, which impacts fission gas behavior. BISON therefore models fission gas behavior, with recent efforts extending its capabilities to high burnup fuel behavior to support the increase in fuel utilization. This talk will provide an overview of the fission gas modeling capabilities in BISON and its predicted impact of fuel performance. Then, we will present recent and ongoing efforts to extend BISON's capabilities for high burnup fuel, which relies on lower length scale modeling efforts in part performed in other MOOSE-based applications: MARMOT and Centipede. The accuracy of these models when compared to experimental data will be discussed.

FUSION 3

Modeling Magnetic Confinement Fusion Systems With MOOSE-based Capabilities

Pierre-Clement Simon (Idaho National Laboratory, INL), Casey T. Icenhour (INL), Masashi Shimada (INL),Guillaume Giudicelli (INL), Logan H. Harbour (INL), Derek Gaston (INL), Lin Yang (INL), Helen Brooks (United Kingdom Atomic Energy Agency), Mahmoud Eltawila (University of Illinois Urbana-Champaign, UIUC), April J. Novak (UIUC), Grayson Gall (North Carolina State University, NCSU), Amanda M. Lietz (NCSU), Trevor Franklin (Virginia Commonwealth University, VCU), Lane B. Carasik (VCU)

For fusion to reach its potential as a clean, sustainable, and abundant energy source to mitigate climate change, advanced modeling and simulation need to play a crucial role in accelerating its deployment. Multiphysics, high-fidelity computational tools are essential to understand, model, and quantify the complex interactions between materials performance, plasma and neutron exposure, and engineering processes. MOOSE-based capabilities meet these needs by leveraging the Multiphysics Object-Oriented Simulation Environment (MOOSE) developed by the U.S. Department of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. These capabilities integrate various existing MOOSE capabilities such as heat transfer, thermomechanics, and thermal hydraulics with MOOSE-based applications like Cardinal (neutronics) and TMAP8 (tritium migration analysis program, version 8). Moreover, it contains dedicated capabilities for plasma edge modeling. This comprehensive and modular integration built on the MOOSE framework allows users to perform massively parallel multiphysics simulations, which are essential for the design, safety analysis, and performance evaluation of fusion systems. These capabilities have been demonstrated on plasma facing components, which are under extreme thermal loads, repeated thermal shocks, and irradiation by plasma ions, neutral particles, and high-energy neutrons throughout their lifecycle. Designing components with acceptable lifetime degradation is highly challenging. This effort aims to model the multiphysics environment in which these components operate, thus accelerating their design and evaluation processes. This presentation will cover the current capabilities and showcase preliminary results. We will also discuss how MOOSE-based applications are being utilized in the fusion community to address critical scientific and engineering challenges, ultimately supporting the deployment of magnetic fusion energy as a power source.

Developments and Updates Within the MOOSE Electromagnetics Module to Facilitate Fusion Multiphysics

Casey Icenhour (Idaho National Laboratory, INL), Corey DeChant (INL), Grayson Gall (North Carolina State University, NCSU), Stephanie Pitts (INL), Stephen Novascone (INL), Pierre-Clément Simon (INL), Daniel Schwen (INL), Benjamin Spencer (INL), Davide Curreli (University of Illinois at Urbana-Champaign, UIUC); Kiruba Haran (UIUC), Amanda Lietz (NCSU)

Since its formal addition to the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework in 2022, the MOOSE electromagnetics (EM) module has been successfully utilized in multiple research areas, including low-temperature plasma industrial processing, electric-field assisted sintering, and studies of microwave propagation in materials. More recently, increased

worldwide interest in fusion energy—and subsequent need for integrated modeling and simulation capabilities within that community—has led to applications of the module in new and exciting areas. This has included fusion magnet technology and scrape-off layer plasma physics models, which has led to new electromagnetics formulations, boundary conditions, and verification and validation exercises. This presentation serves as a showcase of these new developments, and an opportunity to share future development plans and goals.

Platypus on the Device: Results and Lessons from GPU Acceleration

Henrique Bergallo Rocha (UK Atomic Energy Authority, UKAEA), Alexander I. Blair (UKAEA), Kingsley Collie (UKAEA), Andrew Davis (UKAEA), William Ellis (UKAEA), Chris MacMackin (UKAEA), Nuno Nobre (UKAEA), Seimon Powell (UKAEA), Edward Palmer (UKAEA)

In the (pre-)Exascale paradigm, GPU acceleration is becoming near-ubiquitous, due to it offering important advantages in terms of compute performance and efficiency. Nonetheless, the present landscape of Finite Element Method (FEM) Multiphysics tools is largely not yet ready to leverage GPU-accelerated architectures. This presents a challenge to the fusion industry in the form of generating qualification data for components, modelling future reactors and existing experiments. A different presentation in this workshop introduces Platypus: a MOOSE app for simulating multiphysics systems using the FEM approach in large-scale engineering with complex geometry, with the intent of utilising MPI parallelism and GPU acceleration for scalability in High-Performance Computing systems. It does so by utilising MFEM as an alternative FE backend to MOOSE's default libMesh. This backend switch allows for supporting GPU acceleration and high-order finite elements spanning the de Rham complex. This presentation describes the different stages of optimising Platypus for running on a CUDA backend, the specific bottlenecks that had to be addressed and how these were tackled. We also present results contrasting Platypus' GPU performance to equivalent CPU runs at different assembly levels, as well as with pre-optimisation runs. Finally, the scaling properties of representative examples are discussed, including multi-node Device runs, thereby demonstrating Platypus' suitability for leveraging the compute capabilities of large-scale GPU clusters.

FRAMEWORK 2

Prelude to Simulation Diagnostics in MOOSE: Diagnosing Meshes

Daniel Yankura (Idaho National Laboratory, INL), Guillaume Giudicelli (INL)

As finite element simulations increase in complexity, so does the need for high quality meshes. Without proper diagnostics, issues pertaining to poor mesh quality or improper mesh construction may go undetected, causing simulations to fail unexpectedly. This paper details the new mesh diagnostic system available in MOOSE, which provides users with the tools to inspect mesh quality for both externally and internally generated meshes. This system can detect issues arising from element volume size, non-conformal elements, intersecting edges, missing sidesets, as well as

other common mesh issues. As meshes increase in size and complexity, such issues become more difficult to diagnose through visual inspection alone.

Physics and Components Syntax for a Systems-Based Approach to Multiphysics

Guillaume Giudicelli (Idaho National Laboratory)

Simulations in MOOSE have traditionally used kernel and boundary condition classes to describe the equations. Downstream applications leveraged a system called Actions to define a pre-packaged discretization of the equations they solve. Unfortunately, the Action base class was very limited, and most applications implemented the same concepts in their Actions. This led to an increased maintenance burden and a reduction in coupling opportunities, save for the use of MultiApps which renders each input mostly independent. With the introduction of multi-system capabilities in MOOSE, there is growing interest in defining entire simulations of complex multiphysics systems in a single input file. By introducing a new Physics system, with its dedicated syntax and a new base class providing wide-ranging capabilities, we are now able to define multiple equations in a single input file in a compact and user-friendly way. With new interactions between Physics and the Component system, these equations can be defined on each component of a complex system. In this talk, we will present the capabilities of these new systems, their interactions, and how to define complex systems multiphysics simulations with Physics and Components.

Integrating Accelerators Into MOOSE

Alexander Lindsay (Idaho National Laboratory)

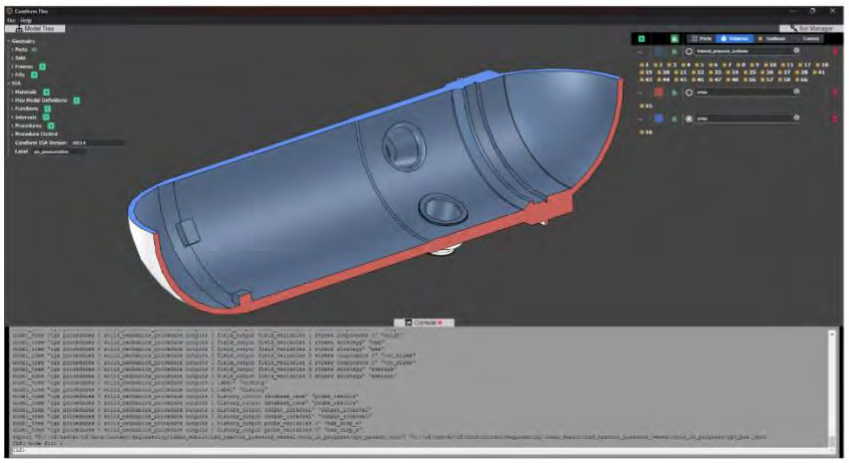
The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a general purpose open source multiphysics framework supporting native finite element and finite volume discretizations that can also wrap other libraries providing arbitrary computational capabilities such as OpenMC and NekRS. Due to its generality, it has experienced significant success. However, with recent changes in the landscape of computer architectures, most notably the growth of Graphical Processing Unit (GPU) computing, MOOSE must assess new technologies or else risk alienating customers interested in the benefits these technologies can offer. In that vein we have assessed multiple accelerator libraries developed through the Exascale Computing Project (ECP) project, including Kokkos, libCEED, and Modular Finite Element Methods (MFEM), and present our evaluation of these libraries as candidates for incorporation into the MOOSE framework.

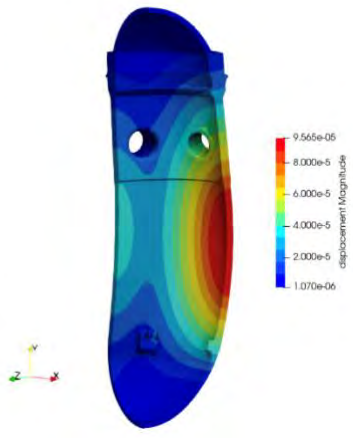
Isogeometric Analysis in MOOSE

Matthew Sederberg (Coreform LLC), Robert Carlsen (Coreform), Greg Vernon (Coreform), Derek Thomas (Coreform), Roy Stogner (Idaho National Laboratory), Greg Vernon (Coreform)

Coreform has collaborated with Idaho National Laboratory to add initial isogeometric analysis (IGA) capabilities to MOOSE. In this presentation, we will demonstrate how to access this from user workflow, setting up a CAD model in Coreform Flex and sending to MOOSE for simulation

without creating a conformal mesh. We will also introduce the concept of isogeometric analysis and share examples of usage from other industries.





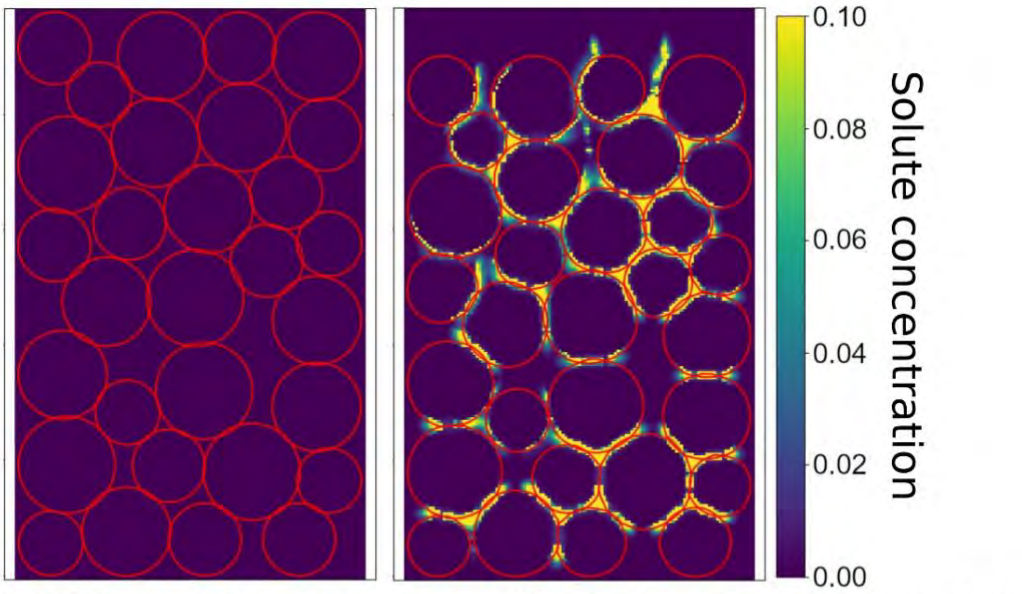
GEOSCIENCE 3

Combine the Phase-Field Description with a Discrete Element Method to Model Chemo-Mechanical Couplings (Pressure-Solution)

Alexandre Sac-Morane (Duke University & UCLouvain), Manolis Veveakis (Duke University), Hadrien Rattez (UCLouvain)

Pressure-Solution plays a pivotal role in a number of geological processes, including the nucleation and recurrence of earthquakes, as well as diagenetic processes. It involves three chemo-mechanical processes at the level of the grains: dissolution due to stress concentration at the contacts, diffusive transport of the dissolved mass from the contact to the pore space, and precipitation of the solute on the less stressed surface of the grains. This mass transfer results in a time-dependent compaction of the granular sample, which is manifested in changes to the microstructure, grain shapes, pore structure and composition. In light of the porous matter's consideration as a multi-phase sample, composed of one phase per grain, the Phase-Field (PF) description emerges as a promising candidate to capture the localized phase transitions (dissolution/precipitation) that occur during this phenomenon. Indeed, the free energy of the Allen-Cahn formulation on the phase variables describing the grains can be tilted based on the local values of the solute concentration in the pore fluid, on the solid activity computed with the stress transmitted and on the kinetic of the dissolution/precipitation. A coupled diffusive equation on the solute concentration is added to account for the mass flux in the fluid and to guarantee the mass conservation. Nevertheless, this continuous scheme is unable to account for the reorganization of the grains, which in turn affects the microstructure of the granular sample. Indeed, the mechanical steady-state is destabilized by the shape evolution of the grains. The Phase-Field theory is then coupled with a Discrete Element Method (DEM). Indeed, this theory considers the individual particles and their interactions, solving Newton’s laws for each grain and assuming penalization laws at the contacts to avoid interpenetration. This theory has recently been extended to capture the irregular shape observed for real particles. The complex shapes of the grains exert a significant

influence on the macroscopic mechanical behavior of the material. Consequently, accurate models should aim to capture this complexity. The coupling between PF and DEM enables the simulation of the irregular shapes of particles in a granular material and their heterogeneous change using the phase-field variable as a particle's geometrical descriptor. The objective of the granular sample is to attain mechanical equilibrium, despite the disturbance caused by the evolution of particle shapes. After some calibration on indentation experiments and validation through two limiting scenarios, the method is applied to build a numerical twin of real oedometric experiments considering several grains.



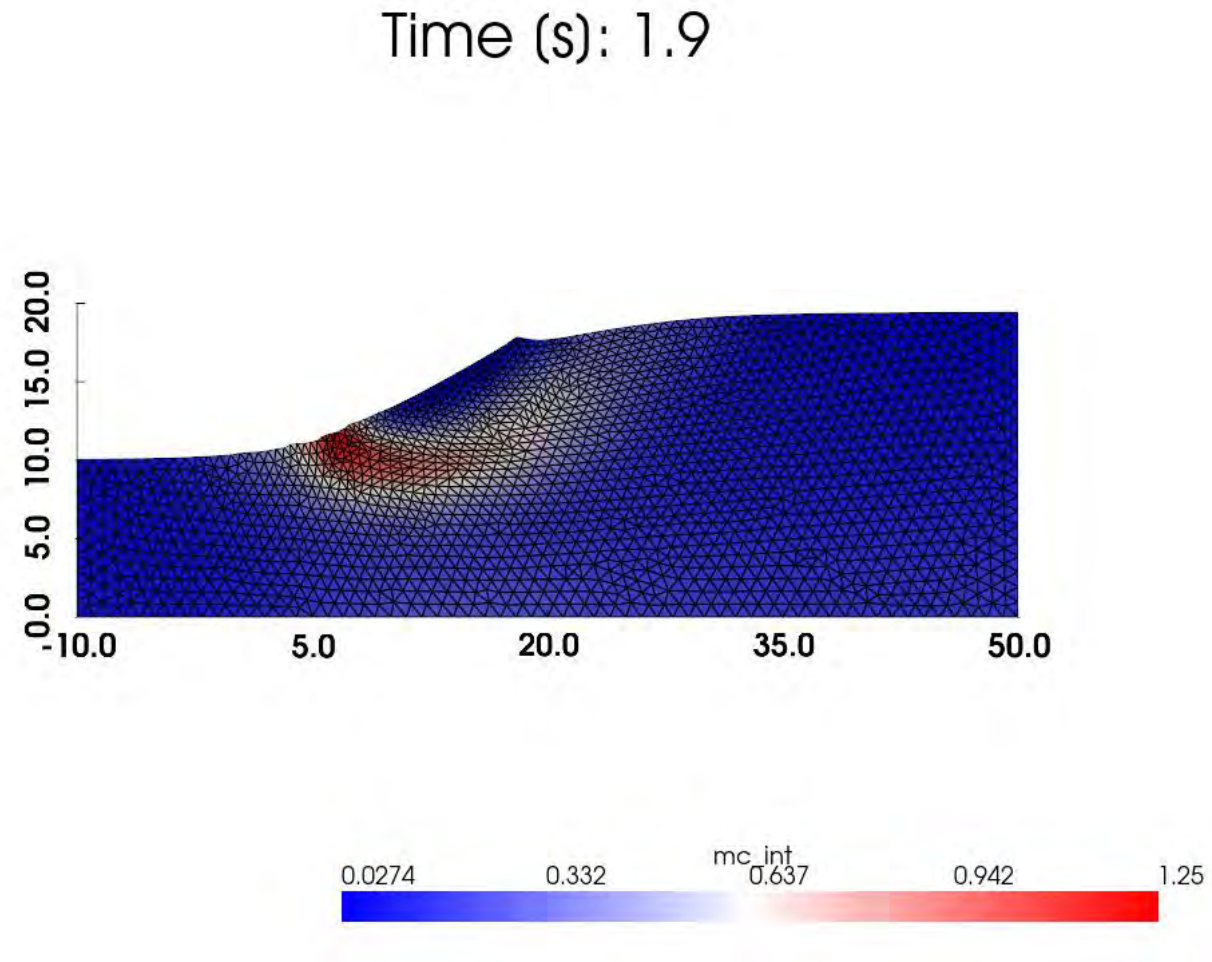
Initial and final configurations (grains and solute) during an oedometric test. The settlement is only du to pressure-solution.

PFEM to Simulate Earthen Dikes Failure Due to Overtopping: A Coupled Surface-Subsurface Approach

Nathan Delpierre (UCLouvain), Hadrien Rattez (UCLouvain), Sandra Soares-Frazao (UCLouvain)

The majority of breaching of earthen embankments is triggered by overtopping flows or waves. With the increasing frequency of extreme precipitation events due to climate change, this type of failure will happen more often in the future. These failure mechanisms are usually simulated using the shallow-water equations complemented by the Exner equation to reproduce the progressive erosion of the embankment and the growth of the breached area. The dynamics of breach opening play a major role in the way water rushes into areas that should be protected by dams or dikes. This is why numerical models have been developed with the aim of making better predictions of breach outflows. Such an approach usually neglects the effect of the degree of water saturation in the embankment as well as the flow through the embankment that can alter the slope stability of this

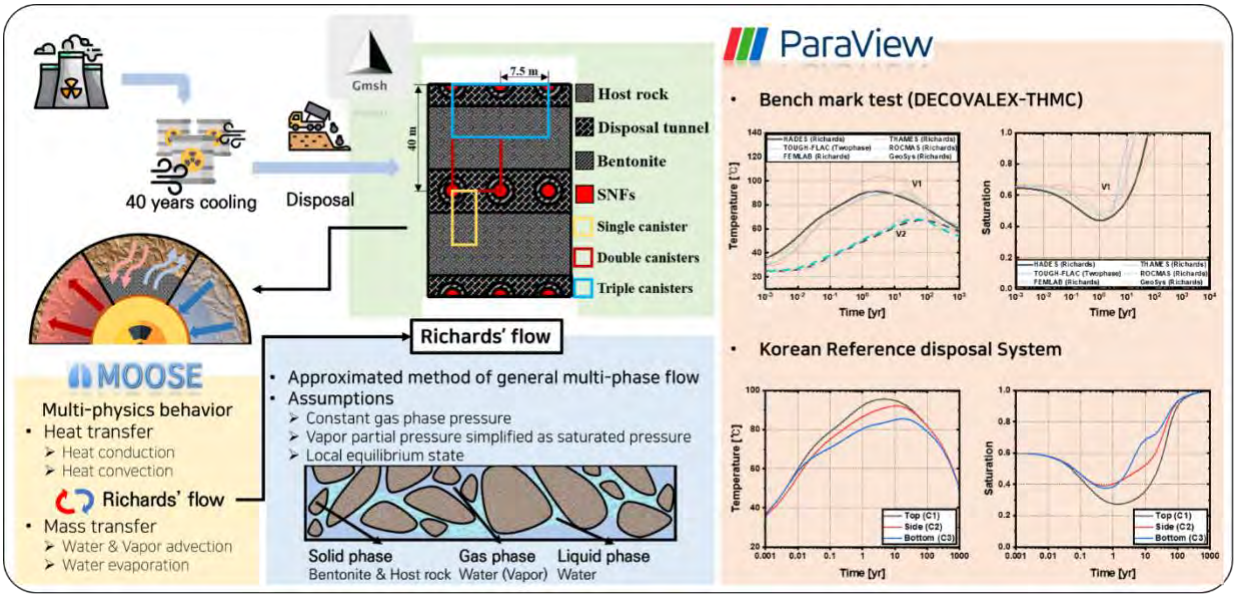
structure by reducing the soil's mechanical strength during overtopping. Such slope instabilities greatly affect the breach opening evolution and should therefore be modelled. Here we present a numerical model in which the surface and subsurface flows are coupled with a geomechanical model of the earthen embankment. The Particle Finite Element Method (PFEM) is used to reproduce the large displacements that occur during the slope failure process generated by mechanical strength losses resulting from pore pressure variation and allow the simulation of the entire dike failure process. The groundwater flow is simulated by solving the 2D Richards equation, while the surface flow is simulated by solving the 1D shallow-water equations. The combination of these flows provides information regarding the pore pressure evolution inside the earthen embankment during the overtopping process. This evolution leads to severe decrease of the soil's shear strength and eventually to complete failure. Several test cases were conducted to show the influence of the coupled flows process on the geomechanical failure. The effects of pore pressure fluctuation and of soil's parameters on the geomechanical failure are studied. This work shows that the geomechanical failure should not be neglected in the process of earthen embankment failure simulation.



HADES (High-level Radiowaste Disposal Evaluation Simulator) Development for Performance Assessment of Deep Geological Repository

Samuel Park (Seoul National University, SNU), Nakkyu Chae (Korea Atomic Energy Research Institute), Pilhyeon Ju (SNU), Sungyeol Choi (SNU)

In order to safely dispose of Spent Nuclear Fuels (SNF), performance assessment through numerical simulation is significant due to temporal and spatial limitations. In this study, a new multi-physics numerical simulation code, HADES (High-level rAdiowaste Disposal Evaluation Simulator), was developed by using the MOOSE framework to conduct performance assessments of Deep Geological Repository (DGR), considering mutual relations between multi-physics behavior. The mutual relations including THC-EC (Thermal-Hydraulic-Chemical-Electrochemical) behavior consist of a main (Thermal-Hydraulic) – sub (Chemical-Electrochemical) applications. Each physics component is implemented via new kernels using the Finite Element Method (FEM). In the main application, addressing TH behavior, the behaviors are modeled using two different approaches: (i) the general two-phase approach, considering pressure change in both liquid and gas phase, and (ii) the Richards' flow approach, assuming the gas pressure is constant as atmospheric value. The chemical behavior, dealing with the reactions related to primary mineral dissolution and precipitation involved in copper canister corrosion, is modeled using chemical kinetics. The electrochemical behavior, addressing the corrosion of copper canister, is implemented using the mixed-potential method, considering five different corrosion reactions. The mixed-potential theory assumes that the sum of surface current densities related to these corrosion reactions is zero. Moreover, the mutual relations between THC-EC behavior are implemented. Additionally, Gmsh and Paraview are employed for mesh generation and data analysis, respectively. HADES has been verified and validated through comparisons with benchmark and experimental results from the DECOVALEX and CIEMAT projects, as well as corrosion experiments. The DECOVALEX benchmark was used for verification set under 100℃ of thermal criteria, while the CIEMAT experiment was addressed as validation set for over 100℃ of thermal criteria. Corrosion experiments were employed as validation set for electrochemical behavior of the code. In addition, HADES has been applied to assess current and enhanced disposal concepts based on the KRS (Korea Reference disposal System) condition, with thermal criteria set of below and above 100℃, respectively. When applying the current disposal concept, the peak temperature reached around 95℃ satisfying the current thermal criterion, similar to KAERI (Korea Atomic Energy Research Institute) results. Furthermore, TH behavior under an advanced repository design, considering reduced distance between SNFs, was calculated. The peak temperatures were approximately 103℃ and 111℃ for distances of 6m and 5m, respectively. In terms of copper canister corrosion behavior, the copper canister, with a 5cm thickness, is estimated to endure for at least 1 million years, even under harsh conditions, having higher concentration of sulfide ion [HS-].

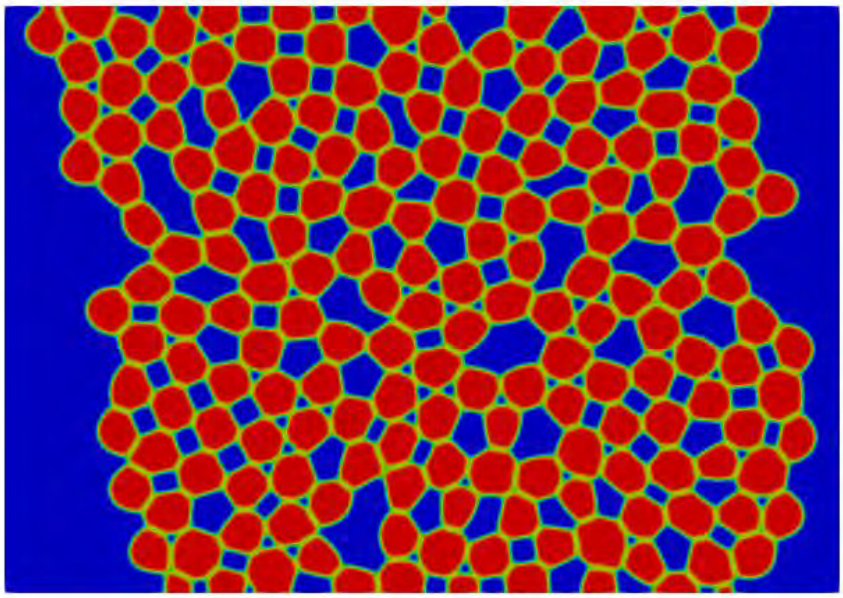


NUCLEAR 6

Phase-Field Simulation of Electric Field Assisted Sintering

Larry Aagesen (Idaho National Laboratory)

A novel electrochemical grand potential functional was introduced to model the electric-field assisted sintering process of an ionic ceramic green body. This phase-field approach allows for the simulation of the consolidation of multiple granular particles and their interactions with surrounding voids. The model considers the effects of charged vacancies and their interactions with both internal and applied electric fields. It also includes defect segregation to grain boundaries and enhanced interfacial defect mobility. Simulations of two-particle systems demonstrated that the influence of the applied electric field on neck growth increased with particle size. A rapid temperature rise was observed at higher field strengths, indicating a flash event in flash sintering. Simulations involving multiple particles revealed that internal Joule heating was concentrated at particle-particle contacts (grain boundaries), despite these areas having lower conductivities than adjacent particle-void interfaces. This resulted in the formation of a percolative path for ionic charge across the green body and the sintered ceramic, accelerating the Joule heating process as the green body's porosity decreased.



Phase Field Modeling of Stress Corrosion Cracking of Structural Alloys in Molten Salt Reactors

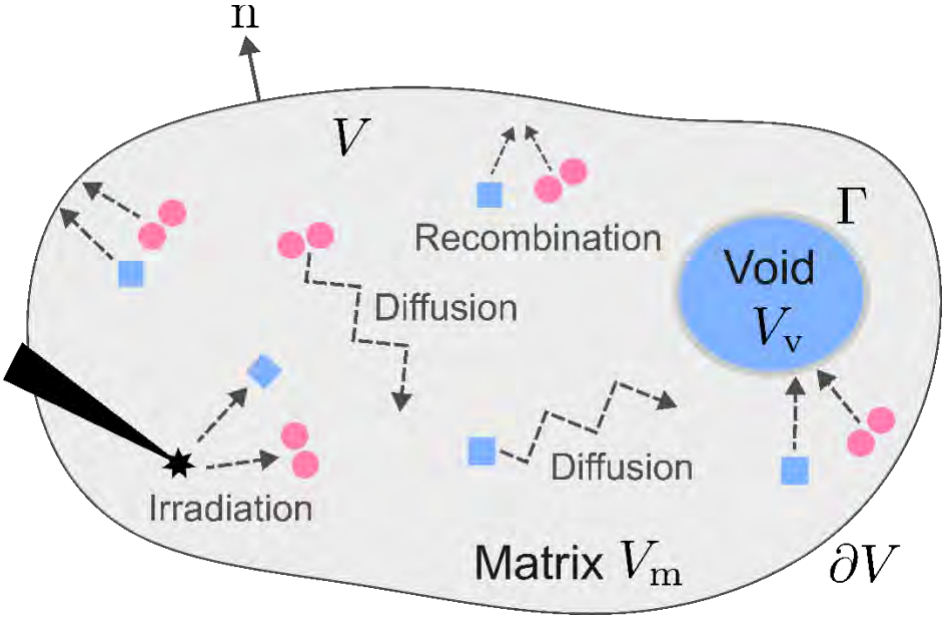
Harsha Pandey (University of Illinois, Urbana-Champaign, UIUC), Lorenzo Vergari (UIUC)

Structural alloys used in Molten Salt Reactors (MSR) are susceptible to corrosion when exposed to molten salts. Even though the chemical reactions between structural alloys and the main constituents of fluoride and chloride salts of interest to reactors are not thermodynamically favored, the presence of impurities within the salt can initiate the oxidation and dissolution of the Cr content in structural material. Additionally, machining irregularities in the alloys with added mechanical and thermal stresses synergistically can lead to environmentally assisted cracking (EAC) phenomena, including stress corrosion cracking (SCC), undermining the durability of structural components. The multi-physics nature of EAC phenomena and the operational complexities in working with molten salts make it challenging to test integral effects experimentally and motivate the development of a computational model that can support and enhance experiments. In this endeavor, modeling of structural alloy corrosion under external stresses in MSRs is realized with the phase-field methodology (PFM) in MOOSE, because of the ability of this approach to successfully capture the multiphysics nature of the problem and also eliminate the mesh dependencies and displacement discontinuities present within other Finite Element Methods by regularizing the solid-salt interface. Metal dissolution and pit propagation are modeled by the Kim-Kim-Suzuki (KKS) model which is employed to minimize the free energy of the system and take into account the contribution of electrochemical energies as well as mechanical energies due to the applied loads. This talk will present the modeling approach developed, its validation strategy, and the interpretation of preliminary results for structural alloy corrosion in FLiBe salt.

Quantitative Phase Field Modeling of Void Growth Under Irradiation in Single-Crystalline Metals: An Accurate Capture of the Thermodynamics of Void Phase

Rayaprolu Goutham Sreekar Annadanam (Purdue University, PU), Kyle Starkey (Materials Design, Inc.), Anter El-Azab (PU)

Existing phase field (diffuse-interface) models for void evolution in solids are not quantitative, in the sense that they do not capture the physics of the sharp interface counterpart. In this work, we introduce a thermodynamically consistent, quantitative phase field model for void evolution in crystalline solids under irradiation. This model considers both vacancies and self-interstitials in the description of void evolution. Unique to this model is fixing the evolution of the non-conserved order parameter describing void surface dynamics by two contributions associated with the interactions of vacancies and interstitials with the void surface by incorporating the two mobility parameters in the corresponding Allen-Cahn equation. In addition, the energetics of the void is formulated to reproduce the Gibbs-Thompson effect, thus distinguishing the current model from the previous models where the chemical potential of a vacancy in the void does not take a correct value, that vary with void size. Asymptotic matching of the phase field model with the sharp-interface theory fixed the two Allen-Cahn mobility parameters in terms of the kinetics of the point defect-surface reactions. The Landau and the gradient coefficients in the free energy construction of the system in its diffuse-interface description are fixed using thermodynamic arguments in terms of the interfacial energy and diffuse interface width. With all the parameters in the phase model clearly expressed in terms of the sharp interface counterparts, we have a novel, quantitative phase field formalism for void evolution in the presence of point defects. To validate this new formalism, several simple test cases were carried out showing the void evolution under simple defect supersaturation scenarios.

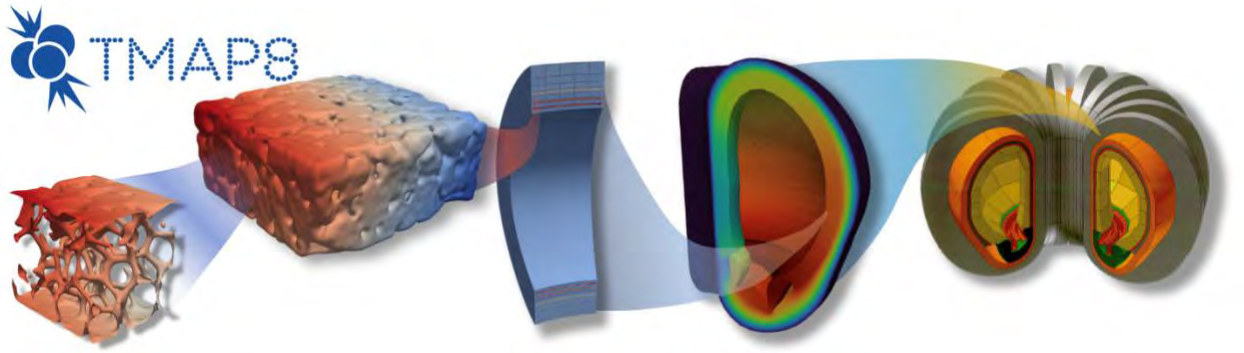


FUSION 4

Verification, Validation, and Demonstration of the MOOSE-Based Tritium Migration Analysis Program, Version 8 (TMAP8) Application for Fusion Systems

Pierre-Clement Simon (Idaho National Laboratory, INL), Casey T. Icenhour (INL), Alexander Lindsay (INL), Gyanender Singh (INL), Chaitanya Bhave (INL), Lin Yang (INL), Adriaan Riet (INL), Paul Humrickhouse (Oak Ridge National Laboratory), Masashi Shimada (INL)

The Tritium Migration Analysis Program (TMAP), developed by Idaho National Laboratory (INL), has been a central tool for analyzing tritium behavior in fusion reactor systems. Previous versions, TMAP4 and TMAP7, facilitated one-dimensional thermal and mass-diffusive transport and trapping calculations. However, their capabilities were limited. For example, both could only model one dimensional domains and were limited in the number of trapping site populations (1 for TMAP4, and 3 for TMAP7). Moreover, they did not easily lend themselves to multiphysics simulations, which limited the accuracy of their predictions. To alleviate these constraints, TMAP8, built on the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework, offers high-fidelity modeling and simulation of tritium transport, enhancing previous capabilities and enabling more efficient design and safety analysis of fusion pilot plants. TMAP4 and TMAP7 capabilities were thoroughly tested in verification and validation (V&V) cases. Following standard engineering terminology, “Verification” is the process of determining that a computational model accurately represents the underlying mathematical model and its solution. “Validation” is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model – requiring comparison against experimental data. TMAP8 has been tested on the same suite of V&V cases to build trust and demonstrate its accuracy in modeling hydrogen isotope transport. These cases are an integral part of the high software quality standards set for TMAP8, which is Nuclear Quality Assurance, Level 1 (NQA-1) compliant. Moreover, TMAP8 is open-source, is thoroughly documented, and uses a flexible license that enables effective collaborations, including public-private partnerships. The TMAP8 online documentation describes all its capabilities, all V&V cases with the associated results and input files, and clear instructions on how to get started. The documentation also includes example and demonstration cases beyond what TMAP4 and TMAP7 were capable of doing, including simulating a complete tritium fuel cycle, two- and three-dimensional tritium migration and heat transfer within a divertor monoblock, pore scale simulations in breeder materials, and others. These cases showcase TMAP8’s ability to retain TMAP4 and TMAP7 essential features while significantly expanding capabilities for complex multiphysics and multiscale analyses on high performance computers. Despite these state-of-the-art capabilities, we will also show that TMAP8 is easy to use and is suitable for different expertise levels.



Evaluating the Impact of Tritium Permeation Membrane Performance and Direct Internal Recycling on Fusion Fuel Cycle Efficiency Using TMAP8

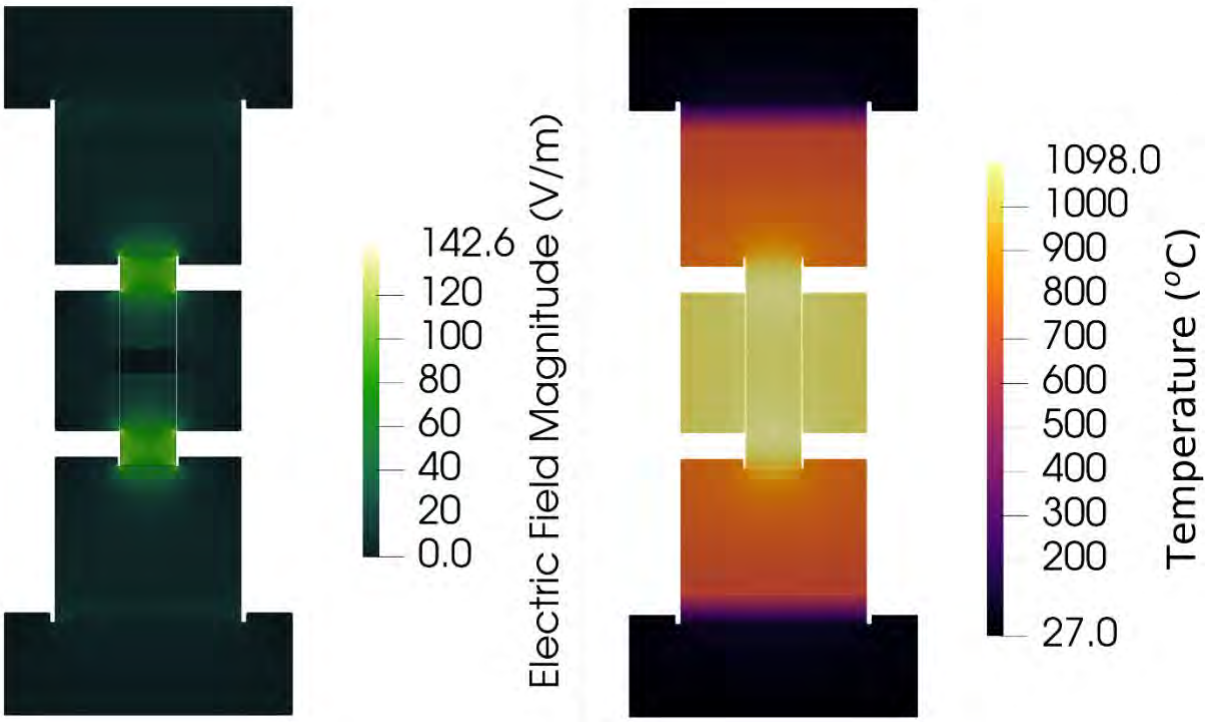
Lin Yang (Idaho National Laboratory, INL), Pierre-Clement Simon (INL), Adriaan Riet (INL), Thomas Fuerst (INL)

An efficient fuel cycle is vital to sustainable and cost-effective energy generation in fusion systems. Since tritium is not widely available, fusion systems must breed their own tritium for sustainable fusion deuterium-tritium reactions. An inefficient fuel cycle increases the tritium inventory needed for operations, which increases costs, constraints on tritium management systems, and safety concerns. A fuel cycle model is a powerful tool for understanding tritium inventories and flow rates across all systems in the fuel cycle. By simplifying the technical details into time-dependent tritium flow rates and inventories, the model can simulate the entire fuel cycle with high computational efficiency, even for technologies that are still under development. It can therefore quantify the impact of new tritium management technologies on fuel cycle efficiency. To evaluate the impact of key components on reducing tritium inventory, we are using and expanding an existing fuel cycle model based on latest advancements in fuel cycle research. The new model integrates Tritium Permeation Membrane (TPM) and Direct Internal Recycling (DIR) to enhance tritium transport from blanket breeders and plasma exhaust. These fuel cycle models are implemented in TMAP8 (Tritium Migration Analysis Program, version 8), a MOOSE-based open-source application designed to provide cutting-edge capabilities for tritium transport and fuel cycle modeling. The study aims to demonstrate the extensibility of existing fuel cycle modeling capability in TMAP8 and to offer a proof-of-principle design for future fusion plant systems. The presentation will cover the performance of fuel cycle modeling capabilities available in TMAP8, highlight advancements in fuel cycle research, and present a sensitivity analysis of these models. The results underline potential approaches and technology solutions to lower tritium inventory requirements, highlighting their role in shaping the future of fusion energy.

Development and Validation of MALAMUTE Simulations for Electric Field Assisted Sintering of Structural Materials

Stephanie A. Pitts (Idaho National Laboratory, INL), Michael J. Moorehead (INL), Larry K. Aagesen (INL), Andrew J. Gorman (INL)

Fusion power plant designs feature extreme material performance requirements for structural material candidates. In addition to conventional alloys, more advanced composites and oxide dispersion strengthened (ODS) alloys are being explored; however, achieving the desired microstructures to maximize performance using traditional manufacturing methods can be challenging. The advanced manufacturing (AM) electric field-assisted sintering (EFAS) technique offers improved control over the final microstructure through faster heating and cooling rates and moderate pressures. Modeling and simulation tools show promise in elucidating the process-structure-property-performance (PSPP) correlation for AM-produced parts, including the EFAS process. An inherently multiscale process, the EFAS technique aligns well with the multiscale modeling capability of the open-source Multiphysics Object-Oriented Simulation Environment (MOOSE). We present here an electro-thermo-mechanical approach to modeling the EFAS process using the MOOSE Application Library for Advanced Manufacturing UTilitiEs (MALAMUTE) code. Prediction of the field and gradient distributions across the EFAS tooling is required to accurately describe the conditions for the lower-scale microstructural evolution models. In this work we show the MALAMUTE model developed to predict the electrical potential, temperature, and mechanical stress distribution across the EFAS graphite tooling and part at the larger engineering-scale. Validation of the MALAMUTE engineering-scale model is completed using data from experimental densification and pre-densified runs of iron powder via EFAS at 1000C. These runs were conducted using a Thermal Technology DCS-5 EFAS system. Data collected during the experiment runs include the direct current (DC) supplied to the graphite tooling, the temperature of the graphite tooling as measured with a pyrometer, the temperature of the rams as measured with thermocouples, and the force applied to the top of the graphite tooling stack. Our validation approach used the current and force data from the EFAS run as boundary condition inputs to the MALAMUTE simulation; the pyrometer data were used to evaluate the MALAMUTE EFAS model prediction. Results of the MALAMUTE simulations are employed to connect the external pyrometer temperature measurement to the temperature profile across the part undergoing consolidation. We investigate the impact of material property variation and mesh deformation on the temperature profile as predicted by MALAMUTE. We conclude by highlighting projects where the MALAMUTE EFAS modeling and simulation capabilities will be used to assist experiment design. Figure: The electric field (left) and temperature (right) predictions from a MALAMUTE simulation of an EFAS pre-densified run of iron during the temperature-hold portion of the manufacturing process.

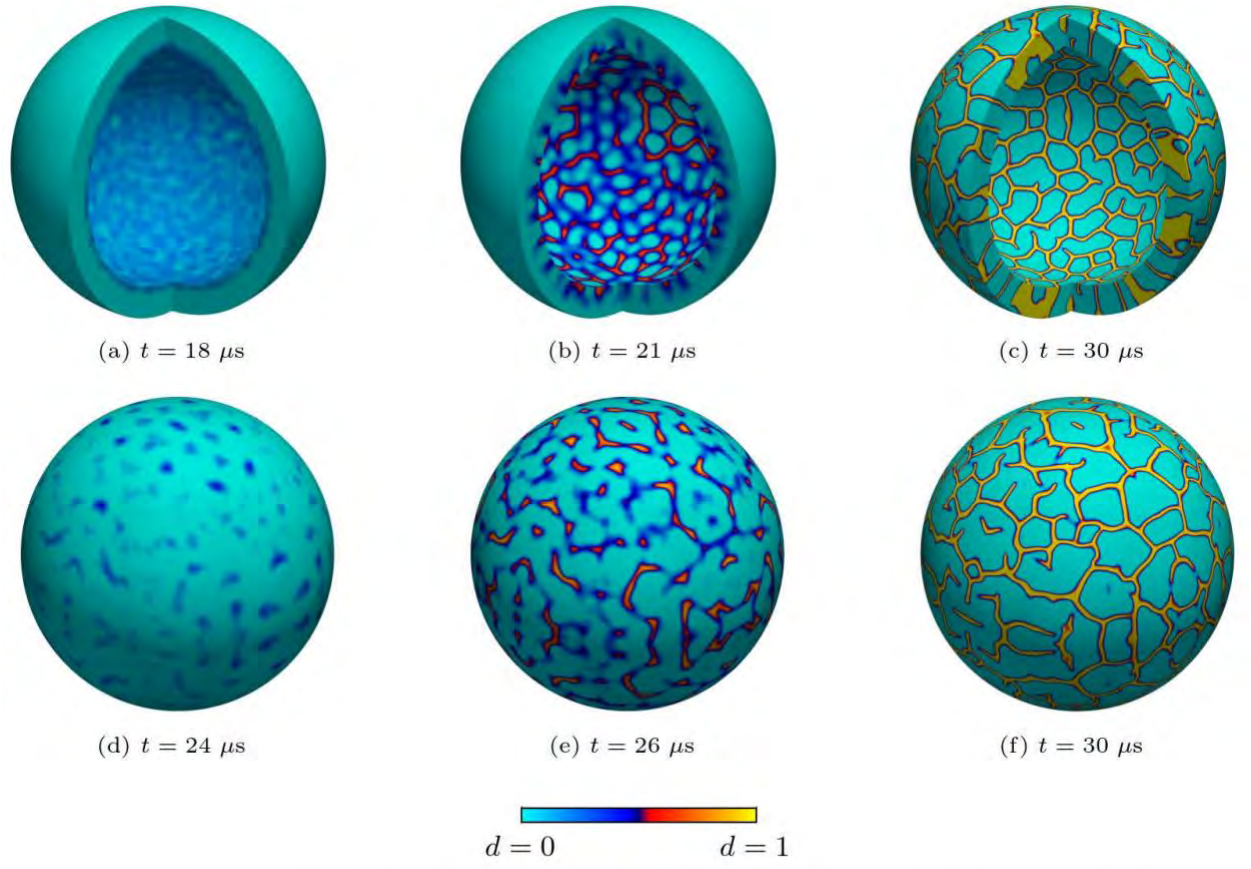


FRAMEWORK 3

RACCOON: A Versatile Framework for Variational Approaches to Fracture with Coupled Field Phenomena

David Esteban Torres (Argonne National Laboratory, INL), Tianchen (Gary) Hu (INL)

Recently, variational approaches to fracture have received great success in solving engineering problems with a wide range of physical phenomena. Designing a unified and flexible computational framework for variational fracture with coupled field phenomena is challenging and has become a strong demand. RACCOON aims to enable such development by providing modular interfaces for each individual physical phenomenon so that implementing the coupling among different phenomena becomes an easy task. Such modular framework, combined with other high-level features of RACCOON, enables rapid development of models for brittle/cohesive/ductile fracture in general nonhomogeneous, anisotropic, dissipative, porous media, optionally coupled with thermal effects, dynamic effects, viscous effects, etc. In addition, RACCOON is developed within the MOOSE framework, which enables capabilities including, but not limited to, dimension-independent programming, automatic differentiation, scaling to a large number of processors, and mesh adaptivity.



Fragmentation of a pressurized hollow sphere modeled using a complete phase-field fracture model.

Hippo: A MOOSE Mulitapp Wrapping OpenFOAM

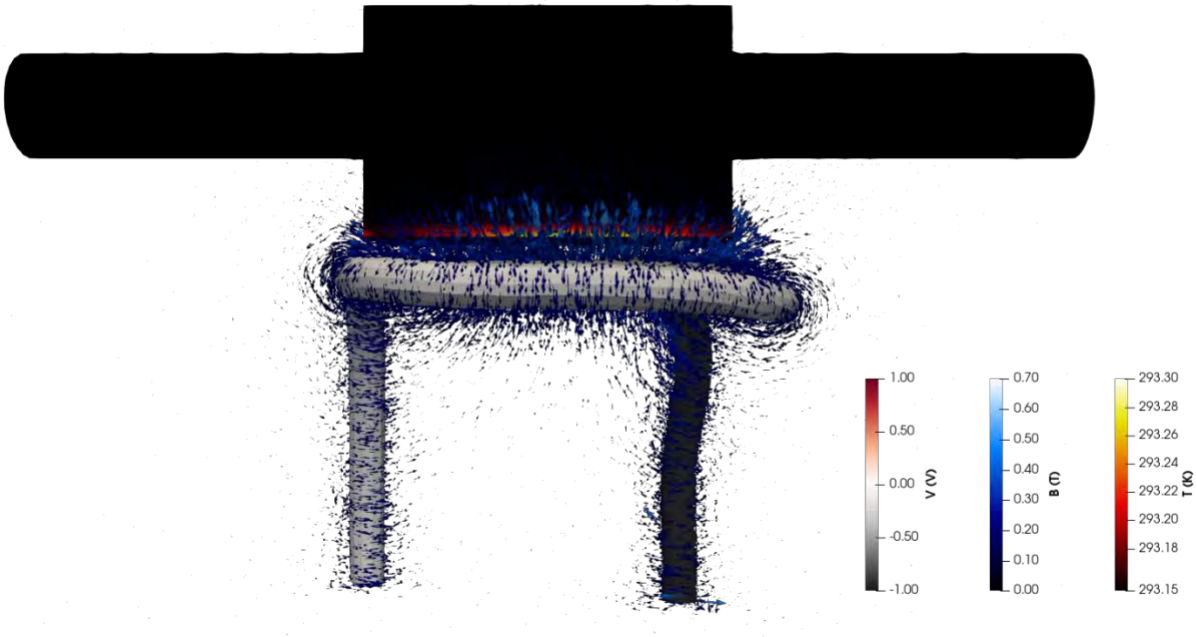
Harry Saunders (UK Atomic Energy Authority, UKAEA), Aleksander Dubas (UKAEA)

Fusion energy research requires modelling Multiphysics problems that involve coupled solid and fluid domains. For example, Tokamak breeder blanket models must be able to calculate the effects of fluid coolants on lithium-bearing materials undergoing neutron heating. MOOSE has thermal and solid mechanics built in and so is an excellent option for modelling solid domains, however it has few turbulence models for fluid domains. A popular option for modelling fluids is OpenFOAM, which is a mature, open source, computational fluid dynamics software that can model complex fluid flow problems and includes a range of turbulence models. MOOSE multiapp Hippo provides a way to solve coupled domain problems using MOOSE and OpenFOAM. Hippo wraps OpenFOAM's buoyantFoam solver and provides tools to solve coupled conjugate heat transfer problems using MOOSE's Transfers system. This software has been used to reproduce results from coupling library preCICE and further testing is underway with complex conjugate heat transfer problems. Future work is planned to support more OpenFOAM solvers and make setting up coupled problems easy for those more familiar with MOOSE and less familiar with OpenFOAM. This tool has the potential to be used in a wide variety of problem domains and provides a way for the MOOSE ecosystem to interface with the robust fluid dynamic solvers in OpenFOAM.

Levelling Up the Support for H(curl) and H(div) Spaces in MOOSE

Nuno Nobre (STFC Hartree Centre, STFC), Karthikeyan Chockalingam (STFC), Sohail Rathore (STFC), Alex I. Blair (UK Atomic Energy Authority)

The solution of scientific problems using finite element methods in MOOSE hinges on robust support for the function spaces of interest in libMesh, its backend discretization library. In this presentation, we will describe the current implementation of H(div)-conforming Raviart-Thomas elements of the lowest order in libMesh, along with the necessary Piola transformation and orientation considerations. This capability has completed the de Rham complex for linear sequences for the first time in libMesh and MOOSE, unlocking new finite element formulations, such as in fluid mechanics for the Darcy saddle point problem, or in electromagnetics for the accurate and efficient representation of current and magnetic flux densities. However, the algebraic systems arising from such formulations often exhibit poor conditioning. To address this issue, we have integrated support for new hypre preconditioners in libMesh. These are the auxiliary-space Maxwell and divergence solvers for H(curl)- and H(div)-conforming spaces, respectively. We will show the performance improvements achieved compared to direct solvers based on LU and Cholesky factorizations for induction heating and magnetohydrodynamics problems relevant to fusion reactor component testing and prototyping settings.



Platypus: A MOOSE Application Enabling FE Problem Assembly and Solution on GPU Architectures using MFEM

Alexander Blair (UK Atomic Energy Authority, UKAEA), H. Bergallo Rocha (UKAEA), K. Collie (UKAEA), A. Davis (UKAEA), W. Ellis (UKAEA), C. MacMackin (UKAEA), N. Nobre (STFC), S. Powell (UKAEA)

Current and upcoming high performance computing systems are increasingly utilising GPU accelerators to augment available compute whilst minimising facility energy requirements. It is of growing importance, therefore, that our simulation tools are capable of effectively leveraging this

available resource on heterogeneous systems in order to maximise performance. Platypus [1] is an open-source MOOSE application that enables finite element problem assembly and solution in parallel on GPU and/or CPU architectures using the MFEM [2] finite element library. By introducing a custom MOOSE Problem type, MFEM objects and wrapped solvers are made available for a range of integrators and finite element types at arbitrary order spanning the de Rham complex whilst maintaining a MOOSE-like interface for the end user to define problems. In this work, we shall present performance results from Platypus at different assembly levels on CPU and GPU devices, along with results from larger scale simulations on complex geometries planned to support upcoming experiments on the HIVE [3] and CHIMERA [4] facilities at UKAEA for fusion-relevant challenges.

1. I. Blair, H. Bergallo Rocha, E. Palmer et al. https://github.com/aurora-multiphysics/platypus
2. R. Anderson, J. Andrej, A. Barker et al. MFEM: A modular finite element methods library, Computers & Mathematics with Applications, 81, (2021)
3. D. Hancock, D. Homfray, M. Porton et al. Testing Advanced Divertor Concepts for Fusion Power Plants Using a Small High Heat Flux Facility, UKAEA Scientific Publications, (2018) https://scientific-publications.ukaea.uk/wp-content/uploads/UKAEA-CCFE-PR23183.PDF
4. T. R. Barrett, C. Carrelli, T. Grant et al. A New Facility for Combined-Load Testing of Fusion Reactor In-Vessel Components, IEEE Transactions on Plasma Science, 48, (2020)

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Thursday, March 13

PLENARIES

Solid Mechanics in MOOSE: History, Nuclear-Energy Applications and Ongoing Development

Ben Spencer, Idaho National Laboratory

The capabilities to model the mechanical deformation of solids have played a key role in MOOSE (the multiphysics object-oriented simulation environment) since its early stages of development. Nuclear fuel performance modeling, through the MOOSE-based BISON code, was an early driver for MOOSE capability development, and remains one of the most important applications of MOOSE. The behavior of nuclear fuel under irradiation is strongly affected by mechanical deformation, fracture, and contact between materials. To meet the need to accurately simulate these phenomena, foundational capabilities were developed in the SolidMechanics and Contact modules. Later efforts to incorporate advanced fracture-mechanics models into fuel-performance modeling resulted in the XFEM and Peridynamics modules. The needs for solid-mechanics capabilities for nuclear energy extend beyond nuclear fuel. The safety of nuclear reactors depends

heavily on the integrity of a variety of structural components, such as reactor vessels, secondary containment vessels, and internal structures that make up the reactor core. These components can experience harsh environmental conditions, and characterizing their susceptibility to failure through numerical simulation is important for ensuring their safety. Component performance, modeled by the Grizzly and BlackBear codes, is important both for the currently operating light water reactors and for the advanced reactors currently being developed for future deployment. Although the materials and conditions differ substantially across reactor types, simulations of component performance rely on common simulation features, such as models for volumetric change, creep, plasticity, damage, fracture, and material degradation, all in a simulation environment that permits coupling with models for other physical phenomena that influence degradation processes. Development to model these phenomena has significantly influenced the MOOSE modules. The mechanics-related modules in MOOSE have undergone multiple major revisions over their lifetimes, and understanding their history and the drivers for their development can help current users and developers of these modules understand their design. In addition to providing an overview of nuclear-energy applications that motivated their development, this talk summarizes some unique architectural features of these modules and discusses current and future development.

Rapid Model Development and Execution With MOOSE

Daniel Schwen, Idaho National Laboratory

MOOSE uses object oriented design principles to make it easy for developers to build on and extend the capabilities of the framework. This presentation reviews some maybe lesser known features of MOOSE that should make life easier not just for developers but also for users of the framework that might not want to delve deep into code development. We will also briefly touch on the question of how slow MOOSE really is and will discuss an ongoing development to accelerate mesoscale modeling with MOOSE(-based applications).